IUPAC-NIST Solubility Data Series. 80. Gaseous Fluorides of Boron, Nitrogen, Sulfur, Carbon, and Silicon and Solid Xenon Fluorides in all Solvents

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The literature has been searched through 2002 June for solubility data on the gases BF_3, NF_3, N_2F_4, SF_6, CF_4, CHF_3, CH_2F_2, CH_3F, C_2F_6, CHF_5, 1,1,1,2-$C_2H_2F_4$, 1,1,1-$C_2H_3F_3$, 1,1-$C_2H_4F_2$, CH_5F, C_3F_8, *c*-C_4F_8, C_2F_4, 1,1-$C_2H_2F_2$, C_2H_3F, C_3F_6, C_3F_6O, and SiF_4 and the solids XeF_6, XeF_4, and XeF_2 in all solvents. The data are compiled here. Where feasible evaluations have been carried out. The evaluations were mostly carried out for water as a solvent as the water systems are the most extensively

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studied. For other systems there is often only one set of measurement or two sets of measurements, which do not agree well. Evaluation of such systems will have to wait on more experimental measurements. © *2005 American Institute of Physics.*
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1. Preface

The present volume of the Solubility Series was started almost 20 years ago. At that time the plan was to include all the gas solubility data in all solvents for all of the gaseous halocarbons. It was soon apparent that this was too many data for one volume. The decision was made to prepare a volume on hydrogen fluorocarbons, HFCs, and add other low boiling and volatile fluorine containing compounds. Thus, in addition to some 16 fluorocarbons there are data on xenon fluorides, trifluoroborane, nitrogen fluorides, sulfur fluoride and tetrafluorosilane. There are other volatile fluorine compounds that could have been included, for example uranium hexafluoride. However, uranium hexafluoride seems to have been covered in earlier reviews.

One of our goals is to prepare evaluations of the data we compile. For many of the data presented here there is only one report of data or two reports, which agree poorly. Thus, we have not prepared as many evaluations as in earlier volumes. Where possible we have tried to prepare an evaluation of the solubility in water of each substance, but even here there is not enough concordant data to make this possible for all the fluoride gases.

The volume was nearing completion about 5 years ago when the Solubility Series changed publishers and an entirely new format was required. This meant converting the lay sheets on which many of the manuscript pages had been prepared to a computer format for the *Journal of Physical and Chemical Reference Data*. Thus, there is a five-year delay in publishing the volume. A part of that delay is due to the inefficiencies of the Editor.

The phasing out of chlorofluorocarbon refrigerants and replacing them with HFC refrigerants has resulted in many new solubility papers on the HFC's. Many of these new solubility data have appeared in the past 5 years and the delay in publication has allowed them to be compiled and appear here.

In compiling and evaluating these data we see new problems for the scientists who measure and use solubility data. One problem is large solubility leading to very concentrated solutions. The traditional point of view of gas solubility leading to dilute solutions needs expanded to very concentrated solutions. This is especially true of the solubility of HFCs in large molecular weight ester lubricating oils with mole fractions of 0.5 or more for the solute gas.

Another problem is the measurement of small solubility values by headspace chromatography. There is no doubt that headspace chromatography is a quick and convenient method of measuring solubility. Numerous papers are appearing with up to 50 or more solvents studied. An inspection of these data indicates a larger uncertainty and sometimes poorer agreement among laboratories than by traditional time consuming methods. Headspace chromatography has the potential to be a reliable method. It is suggested that an international committee study the method and propose a procedure and test systems that will insure more precise and accurate results.

Every effort was made to have complete coverage of the literature through June 30 2002. A few more recent papers are included. Some of the solubility data are reported, to the chemist's mind, in obscure engineering journals and in Government reports that may not have been completely abstracted. We know we have missed some of these. We would appreciate having missed papers called to our attention.

The editor wants to express his appreciation to the students of Rubin Battino at Wright State University, Justin Bohrer and Frank Campanell, who conducted a much needed literature search of the most recent 15 years for the volume. Also appreciated was the help of Professor Hiroshi Miyamota who obtained and partially translated several Japanese papers. However, the editor takes responsibility for all missed papers.

Figures on page 019 from the *Journal of Physical Chemistry*; on page 020 from *Journal of Chemical and Engineering Data* and on page 050 from *Analytical Chemistry* were used with the permission of the copyright holder, The American Chemical Society.

H. Lawrence Clever
Atlanta, Georgia 30322
June 2003

2. Introduction to the Solubility Data Series. Solubility of Gases in Liquids

2.1. Nature of the Project

The Solubility Data project (SDP) has as its aim a comprehensive review of published data for solubilities of gases, liquids and solids in liquids or solids. Data of suitable precision are compiled for each publication on data sheets in a uniform format. The data for each system are evaluated and, where data from different sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values, and compiled data sheets are published on consecutive pages.

2.2. Compilations and Evaluations and Quantities and Units Used in Compilation and Evaluation of Solubility Data

Formats for the compilations and critical evaluations have been standardized for all volumes, and complete details for these formats can be found in the *Introduction to the Solubility of Gases in Liquids* published in previous *Solubility Data Series* volumes, for example, Fogg *et al.*[1]

Solubilities of gases in liquids have been the subject of research for a long time, and have been expressed in a great many ways. The nomenclature, use of symbols and units in the IUPAC-NIST Solubility Data Series follow, where possible, Mills,[2] again reviewed in detail in Fogg *et al.*[1] A few quantities follow the ISO standards[3] or the German standard;[4] see a review by Cvitaš[5] for details. Very complete and updated definitions on nomenclature and use of symbols and units has been published in a recent review by Lorimer.[6]

A note on nomenclature. The nomenclature of the IUPAC *Green Book*[2] calls the solute component B and the solvent component A. In compilations and evaluations, the first-named component (component 1) is the solute, and the second (component 2 for a two-component system) is the solvent. The reader should bear these distinctions in nomenclature in mind when comparing equations given here with those in the *Green Book*. Additional details can be found in the review of Lorimer.[6]

2.3. References for the Introduction to the Solubility of Gases in Liquids

[1] P. G. T. Fogg, S.-W. Annie Bligh, M. Elizabeth Derrick, Y. P. Yampol'skii, H. L. Clever, A. Skrzecz, and C. L. Young, *Solubility of Ethyne in Liquids*, IUPAC-NIST Solubility Data Series, Vol. 76, J. Phys. Chem. Ref. Data **30**(**6**), 1693 (2001).

[2] I. Mills *et al.*, eds., *Quantities, Units and Symbols in Physical Chemistry* (the *Green Book*) (Blackwell Scientific Publications. Oxford, U.K. 1993).

[3] ISO Standards Handbook, *Quantities and Units* (International Standards Organization, Geneva, 1993).

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3. Critical Evaluations and Compilations of Solubility Data

3.1. The Xenon Fluorides

Components:	**Evaluator:**
(1) Xenon fluorides;	Bruno Jaselskis,
XeF_2; [13709-36-9]	Department of Chemistry,
XeF_4; [13709-61-0]	Loyola University of Chicago,
XeF_6; [13693-09-9]	6525 North Sheridan Road,
(2) Various inorganic and organic solvents	Chicago, IL 60626

Critical Evaluation

An evaluation of the solubility of the xenon fluorides, XeF_2, XeF_4, and XeF_6, in a number of inorganic solvents

General Remarks

The xenon fluorides are prepared and stored in copper or nickel apparatus using a vacuum line. Only xenon difluoride can be stored in dry glass. All of the xenon fluorides are powerful oxidizing and fluorinating agents and their oxidizing and fluorinating power increase with the increasing oxidation state of the xenon. Solutions are prepared by weight on a vacuum line using, either polychlorotrifluoroethane (Kel-F) or Teflon, and either copper or nickel apparatus. Because of the experimental difficulties the available solubility data are sparse, and a critical evaluation of the data is impossible. For the most part the data must be accepted as they stand.

The melting points and several vapor pressure values[4] are:

Substance	Melting point (T/K)	Vapor pressure (p_1 /kPa, at T/K)			
		293.15	295.82	298.15	373.15
XeF_2	413.2	—	—	0.51	42.4
XeF_4	387.2	0.4	—	—	—
XeF_6	319.2	2.7	3.124	—	—

Xenon Fluoride; XeF_2; [13709-36-9]

1. XeF_2+H_2O; [7732-18-5]

Three papers reported the solubility of XeF_2 in H_2O at 273 K.[1–3] The agreement among the three papers is satisfactory and a solubility of 0.150 mol L^{-1} is accepted as a tentative value. The evaluator judges the value to have an uncertainty of about ±5%.

Aqueous solutions of XeF_2 are unstable, a slightly acidic solution decomposes with a half life of about 7 h at 273 K. In the presence of HF the decomposition is faster, and the rate constant is a function of the HF concentration.

2. XeF_2+HF [7664-39-3]

Hyman and Quaterman[4,5] report the solubility of XeF_2 in pure anhydrous HF at three temperatures. There are no other data to compare with these. The solutions are non-conducting and stable over the 271–303 K temperature interval with an enthalpy of solution of 10.5 kJ mol^{-1}.

3. XeF_2+NOF; [7789-25-5]+HF; [7664-39-3] (NOF·3HF)

Nikolaev *et al.*[6] report the solubility of XeF_2 at several temperatures in a mixed solvent of 1 mol NOF to 3 mol HF. The enthalpy of solution from the solubility values is 8.4 kJ mol^{-1}. There are no other values to compare.

4. XeF_2+IF_5; [7783-66-6]

Nikolaev *et al.*[7] report five solubility values between 288 and 343 K with an enthalpy of solution of (17±7) kJ mol^{-1}. The uncertainty of the enthalpy is a result of the scatter in the solubility values. Sladky and Bartlett[8] report XeF_2 reacts with IF_5 with gas evolution to produce adducts of $XeF_2 \cdot IF_5$. They isolated and characterized the adduct. These observations are not consistent and cannot be resolved with our present knowledge. Nikolaev *et al.*[7] point out the decreasing solubility with solvent in the series: NOF·3HF>HF>IF_5.

5. XeF_2+CH_3CN; [75-05-8]

Meinert and Rudinger[9] report values of the solubility of XeF_2 in CH_3CN at 273 and 294 K. The enthalpy of solution is 7.2 kJ mol^{-1}. The XeF_2 in the pure dry acetonitrile (purified by the method of Coetzes *et al.*[10] is stable at 263 K. The solution can be stored for a prolonged time under this condition.[11] The solution stability depends on the temperature, the purity and the water content of the acetonitrile.

6. XeF_2+UF_6; [7783-81-5]

Nikolaev and Sadikova[12] reported one value of the solubility of XeF_2 in UF_6 at (373±5) K.

7. XeF_2+Other Solvents.

Table 1 summarizes the qualitative observations on the behavior of XeF_2 in a number of inorganic and organic solvents. No data sheets were prepared for these systems.

Xenon fluoride; XeF_4; [13709-61-0]

1. XeF_4+HF [7664-39-3]

Hyman and Quaterman[4,5] report the solubility of XeF_4 in pure anhydrous HF at several temperatures. The solutions are non-conducting and stable over the 271–303 K temperature interval. The enthalpy of solution is 28.0 kJ mol^{-1}. There are no other data to compare with these.

2. XeF_4+NOF; [7789-25-5]+HF; [7664-39-3] (1 NOF: 3 HF)

Nikolaev *et al.*[6,7] report the solubility of XeF_4 between 291.6 K and 354.1 K in a mixed solvent of 1 mol NOF to 3 mol HF. The solubility is greater in the mixed solvent than in the pure HF. The estimated enthalpy of solution is > 20.1 kJ mol^{-1}.

3. XeF_4+IF_5; [7783-66-6]

Nikolaev *et al.*[7] report six solubility values between 296.2 K and 343 K. The solubility values are greatly scattered and the estimated enthalpy of solution from the solubility data ranges from 6 to 30 kJ mol^{-1}.

Table 2 summarizes the qualitative observations on the behavior of XeF_4 in a number of inorganic and organic solvents. No data sheets were prepared for these systems.

Xenon fluoride; XeF_6; [13693-09-9]

1. XeF_6+HF; [7664-39-3]

Hyman and Quaterman[4,5] reported the solubility of XeF_6 in pure anhydrous HF at four temperatures between 289.0 K and 303.4 K. The XeF_6 reacts to form complex ions and the solution conductivity increases with concentration. The enthalpy of solution is 75 kJ mol^{-1}.

References:

[1]E. H. Appelman and J. G. Malm, J. Am. Chem. Soc. **86**, 2297 (1964).

[2]E. H. Appelman, Inorganic Chem. **6**, 1268 (1967).

[3]A. V. Nikolaev, A. A. Opalovskii, and A. S. Nazarov, Dokl. Akad. Nauk SSSR **181**, 361 (1968).

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[18]J. H. Holloway and R. D. Peacock, Proc. Chem. Soc. 389 (1962).

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TABLE 1. Qualitative observations on the solution behavior of XeF_2 in a number of inorganic and organic solvents

Solvent	Remarks	Reference
Sulfur dioxide; SO_2; [7446-09-5]	Quite soluble in the 201–263 temperature interval.	13
Dimethylsulfoxide; $(CH_3)_2SO$; [67-68-5]	Soluble but reacts with gas evolution; solutions are colorless.	13
Liquid ammonia; NH_3; [7664-41-7]	Sparingly soluble in the range 195–263 K and forms NH_4F.	13
Difluorodichloromethane; CCl_2F_2; [75-71-8]	No reaction.	13
Chlorotrifluoromethane; $CClF_3$; [75-77-9]	Sparingly soluble up to the normal boiling point.	13
1, 3-Dioxane; $C_4H_8O_2$; [505-22-6]	Dissolves and reacts.	14
1, 4-Dioxane; $C_4H_8O_2$; [123-91-1]	Dissolves and reacts.	14
Pyridine; C_5H_5N; [110-86-1]	Dissolves and reacts.	14
Dimethylformamide; C_3H_7NO; [68-12-2]	Dissolves and reacts.	14
Tetrahydrofurane; C_4H_8O; [109-99-9]	Dissolves and reacts.	14
Nitromethane; CH_3NO_2; [75-52-5]	Dissolves and reacts.	14
Tetrachloromethane; CCl_4; [56-23-5]	Sparingly soluble.	14
Trimethylphosphate; $(CH_3O)_3PO$; [512-56-1]	Dissolves at room temperature; forms quite stable solution.	14
Diphenylphophinic chloride; $(C_6H_5)_2P(O)Cl$; [1499-21-4]	Dissolves at room temperature; forms quite stable solution.	14
Hexamethylphosphoric acid triamide; $[(CH_3)_2N]_3P(O)$; [680-31-9]	Dissolves; solutions stable up to 323 K.	14
Arsenic trifluoride; AsF_3; [7784-35-2]	XeF_2 reacts.	15
Bromine trifluoride; BrF_3; [7787-71-5]	Dissolves without apparent decomposition.	15
Iodine pentafluoride; IF_5; [7783-66-6]	Dissolves with gas evolution.	15
Trifluoroacetic acid; CF_3COOH; [76-05-1]	Reacts to form $FXeO_2CF_3$.	16

TABLE 2. Qualitative observations on the solution behavior of XeF_4 in a number of inorganic and organic solvents

Solvent	Remarks	Reference
Antimony pentafluoride; SbF_5; [7783-70-2]	Dissolves with gas evolution.	17
Bromine trifluoride; BrF_3; [7787-71-5]	Forms complex species.	17, 18
Acetic anhydride; $(CH_3CO)_2O$; [108-24-7]	Decomposes.	16
Trifluoroacetic acid anhydride; $(CF_3CO)_2O$; [76-05-1]	Dissolves without reaction; no further data.	16
Diethyl ether; $(CH_3CH_2)_2O$; [60-29-7]	Sparingly soluble; decomposes.	18
Dimethylformamide; $HCON(CH_3)_2$; [68-12-2]	Dissolves without decomposition.	16
Acetonitrile; CH_3CN; [75-05-8]	Sparingly soluble.	13, 16
Dimethylsulfoxide; $(CH_3)_2SO$; [67-68-5]	Decomposes.	13, 16
Fluorotrichloromethane (Freon-11); CCl_3F; [75-69-4]	Insoluble.	13
Dichlorodifluoromethane (Freon-12); CCl_2F_2; [75-71-8]	Insoluble.	13
Tetrachloromethane; CCl_4; [56-23-5]	Insoluble.	19

Components:	Original Measurements:
(1) Xenon fluoride; XeF_2; [13709-36-9] (2) Water; H_2O; [7732-18-5]	E. H. Appelman and J. G. Malm, J. Am. Chem. Soc. **86**, 2297–98 (1964).
Variables:	**Variables:**
T/K=273	T/K=273

Experimental Values

The authors report a solubility of 5 mg $(mL)^{-1}$ in water at 0 °C. This corresponds to a solubility of 0.148 mol L^{-1} (compiler).

Auxiliary Information

The authors report xenon difluoride persists in slightly acidic solutions and decomposes at 0 °C to O_2 and HF with a half life of 7 h. The authors used photochemically prepared XeF_2, froze samples of about 0.5 g in liquid nitrogen, pipetted in 20 mL of ice on 20 mL of ice water and brought the system to 0 °C. Sample larger than 25 mg $(mL)^{-1}$ did not dissolve completely.

No other information given.

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Variables:	**Prepared By:**
T/K=273	Bruno Jaselski

Experimental Values

The author's study of the decomposition of XeF_2 in aqueous HF solution started with a saturated solution of XeF_2 which the authors stated was 0.145–0.151 mol L^{-1}.

Auxiliary Information

The xenon difluoride rate of decomposition in aqueous HF increases with the HF concentration, the first order rate constant is a function of the HF concentration in mol L^{-1}. It is:

$$k=(0.313+148c_{HF})\times10^{-4}\,s^{-1}.$$

No other information given.

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$$k=(0.313+148\,c_{HF})\times10^{-4}\,s^{-1}.$$

Components:
(1) Xenon fluoride; XeF_2; [13709-36-9]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. H. Appelman, Inorganic Chem. **6**, 1268–69 (1967).

Variables:
T/K=273

Prepared By:
H. L. Clever

Experimental Values

Solubility of xenon difluoride in water at 273 K

t/°C	T/K	Xenon difluoride solubility (m_1 /mol kg^{-1})
0	273	0.153±0.0015

In other experiments a saturated solution of XeF_2 was found to have a specific conductance of 4×10^{-4} (Ω cm)$^{-1}$ at 273 K. This is about the same specific conductance as a 4.3×10^{-3} mol L^{-1} solution of HF. The author concluded the conductance of XeF_2 solution was due to the HF formed in the reaction:

$$XeF_2+H_2O=Xe+(1/2)O_2+2HF$$

The author concluded that 97% of the dissolved XeF_2 was initially present at molecular XeF_2.

Auxiliary Information

Method/Apparatus/Procedure:
Solid XeF_2 was vacuum distilled into a Kel-F tube. Water at 273 K was added to just form a saturated solution. The saturated solution was analyzed by addition of sulfuric acid and sodium iodide followed by titration with standard thiosulfate solution

Source and Purity of Materials:
(1) Xenon difluoride. Prepared by heating a 10:1 mole mixture of Xe and F_2 overnight at 300 °C in a monel container. Excess Xe removed, 10% of product distilled to remove XeF_4 and the rest vacuum distilled into a Kel-F container.
(2) Water. Nothing specified, but assume double distilled water for the conductivity work.

Estimated Error:
Temperature: Nothing specified.
Solubility: See deviation in table above. The number of determinations not given.

Components:
(1) Xenon fluoride; XeF_2; [13709-36-9]
(2) Hydrogen fluoride; HF; [7664-39-3]

Original Measurements:
H. H. Hyman and L. A. Quaterman, *Noble Gas Compounds*, H. Hyman, ed. (University of Chicago Press, Chicago, IL, 1963), pp. 275–278.

Variables:
T/K=271.2–303.10

Prepared By:
Bruno Jaselskis

Experimental Values

Solubility of xenon difluoride in anhydrous hydrofluoric acid from −2.0 °C to 29.95 °C.

t/°C	T/K	Xenon difluoride solubility (m_1 /mol kg^{-1})
−2.0	271.2	6.38
12.5	285.4	7.82
29.95	303.10	9.88

These data are repeated in Malm *et al.*[1]

The solutions are nonconducting and stable. The enthalpy of solution (van't Hoff) is 10.5 kJ mol^{-1}.

House[2] has calculated the XeF_2 solubility parameter to be δ/J$^{-1/2}$ cm$^{3/2}$=68.2.

Auxiliary Information

Method/Apparatus/Procedure:
Solutions of appropriate concentration were prepared by weight. They were heated slowly and the temperature at which the crystal disappeared was recorded.

Source and Purity of Materials:
(1) Xenon difluoride. Prepared by irradiation of a Xe+F_2 mixture by UV light. Melting point is about 140 °C, vapor pressure at 25 °C is 3.8 mmHg (C. L. Chernick, *The Noble Compounds*, pp 35–38).
(2) Hydrofluoric acid. Redistilled. Conductivity less than 1×10^{-4} s cm^{-1} at 0 °C (Hyman *et al.*[3]).

Estimated Error:
Temperature: Nothing specified.
Solubility: Nothing specified.

References:
[1]T. G. Malm, H. Selig, J. Tortner, and S. A. Rice, Chem. Rev. **65**, 199 (1965).
[2]J. E. House, Jr., J. Fluorine Chem. **22**, 299 (1983).
[3]H. H. Hyman, L. A. Quaterman, M. Kilpatric, and J. J. Katz, J. Phys. Chem. **65**, 123 (1961).

Components:

(1) Xenon fluoride; XeF_2 ; [13709-36-9]
(2) Hydrogen fluoride; HF; [7664-39-3]

Original Measurements:

H. H. Hyman, L. A. Quaterman, *Noble Gas Compounds*, H. Hyman, ed (University of Chicago Press, Chicago, IL, 1963), pp. 275–278.

Variables:

T/K = 293.2–333.10

Prepared By:

Bruno Jaselskis

Experimental Values

Solubility of xenon tetrafluoride in anhydrous hydrofluoric acid from 20 °C to 60 °C

T/°C	T/K	Xenon tetrafluoride solubility (m_1 /mol kg^{-1})
20	293.2	0.18
27	300.2	0.44
40	313.2	0.44
		0.73

These data are repeated in Malm *et al.*[1]

The solutions are nonconducting and stable. The enthalpy of solution (van't Hoff) is 28.0 kJ mol^{-1}.

House[2] has calculated the XeF_4 solubility parameter to be δ/J$^{-1/2}$ cm$^{-3/2}$ = 63.1.

Auxiliary Information

Method/Apparatus/Procedure:

Solutions of appropriate concentration were prepared by weight. They were heated slowly and the temperature at which the last crystal disappeared was recorded.

Source and Purity of Materials:

(1) Xenon tetrafluoride. Heat 1 part Xe with 5 parts F_2 at 400 °C for 1 h. Melting point is about 114 °C, vapor pressure at 25 °C is 3 mmHg. (C. L. Chernick, *Noble Gas Compounds*, pp. 35–38).
(2) Hydrofluoriic acid. Redistilled. Conductivity less than 1 $\times 10^{-4}$ S/cm (Hyman *et al.*[3]).

Estimated Error:

Temperature: Nothing specified.
Solubility: Nothing specified.

References:

[1]T. G. Malm, H. Selig, J. Tortner, and S. A. Rice, Chem. Rev. **65**, 199 (1965).

[2]J. E. House, Jr., J. Fluorine Chem. **22**, 299 (1983).

[3]H. H. Hyman, L. A. Quaterman, M. Kilpatrick, and J. J. Katz, J. Phys. Chem. **65**, 123 (1961).

Components:

(1) Xenon fluoride; XeF_6 ; [13693-09-9]
(2) Hydrogen fluoride; HF; [7664-39-3]

Original Measurements:

H. H. Hyman and L. A. Quaterman, *Noble Gas Compounds*, H. H. Hyman, ed. (University of Chicago Press, Chicago, IL, 1963), pp. 275–278.

Variables:

T/K = 289.0–303.40

Prepared By:

Bruno Jaselskis

Experimental Values

Solubility of xenon hexafluoride in anhydrous hydrofluoric acid from 15.8 °C to 30.25 °C

T/°C	T/K	Xenon hexafluoride solubility (m_1 /mol kg^{-1})
15.8	289.0	3.16
21.7	294.9	6.06
28.5	301.7	11.2
30.25	303.4	19.45

These data are repeated in Malm *et al.*[1]

The xenon hexafluoride reacts to form complex ions, and the solution conductivity increases with concentration.

The enthalpy of solution (van't Hoff) is 75 kJ mol^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:

Solutions of appropriate concentration were prepared by weight. They were heated slowly and the temperature at which the last crystal disappeared was recorded.

Source and Purity of Materials:

(1) Xenon hexafluoride. Heat 1 part Xe with 20 parts F_2 at 300 °C for 16 h. Melting point is about 46 °C, vapor pressure at 25 °C is 29 mm Hg. (C. L. Chernick, *Noble Gas Compounds*, pp. 35–38.)
(2) Hydrofluoriic acid. Redistilled. Conductivity less than 1 $\times 10^{-4}$ S/cm (Hyman *et al.*).

Estimated Error:

Temperature: Nothing specified.
Solubility: Nothing specified.

References:

[1]T. G. Malm, H. Selig, J. Tortner, and S. A. Rice, Chem. Rev. **65**, 199 (1965).

[2]H. H. Hyman, L. A. Quaterman, M. Kilpatrick, and J. J. Katz, J. Phys. Chem. **65**, 123 (1961).

Components:

(1) Xenon fluoride; XeF_2 [13709-36-9]
(2) Nitrosyl fluoride; NOF; [7789-25-5]
(3) Hydrogen fluoride; HF; [7664-39-3]

Original Measurements:

N. S. Nikolaev, A. S. Nazarov, A. P. Opalovskii, and A. F. Trippel, Dokl. Acad. Nauk SSSR **186**, 1331–33 (1969)

Variables:

T/K=290.0–353.2

Prepared By:

Bruno Jasselskis

Experimental Values

Solubility of xenon difluoride in a mixture of one mol NOF and three mol HF at 18.4–80 °C

t/°C	T/K	XeF_2 solubility $100w_1$*	XeF_2 solubility (m_1/mol kg^{-1})
16.8	290.0	73.25, 74.60	16.8±0.8
33.2	306.4	76.82	19.6
49.2	322.4	78.88	22.1
61.0	334.2	78.88	25.4
80.0	334.2	83.80, 84.22	31.0±0.7

*The authors reported g solute per 100 g of solution and the compiler calculated the molal solubility values.

The solutions are nonconducting and stable. The enthalpy of solution (van't Hoff equation) is 8.4 kJ mol^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:

Solutions of appropriate concentration were prepared by weight in a dry box and hermetically sealed in Teflon containers. Temperature was controlled to ±0.2 °C. The saturated solutions were analyzed for nitrogen, fluorine and the amount of xenon tetrafluoride calculated.

Source and Purity of Materials:

(1) Xenon difluoride. Reported purity of 99%.
(2) Nitrosyl fluoride.
(3) Hydrogen fluoride.
The NOF·3HF mixture prepared by the procedure of Steel and Birnkrant.[1,2] The NOF and excess anhydrous HF are mixed at 30–40 °C. The solution is distilled and a fraction boiling at 94–98 °C has the 1 mol NOF 3 mol HF composition. The conductivity is 2400 Ω^{-1} cm^{-1} (i.e., S/cm).

Estimated Error:

Not specified, but can be deduced from two values reported at 16.8 °C and 80 °C, the compiler estimates the reproducibility to be on the order of 2%.

References:

[1]F. Steel and W. Birnkrant, Angew. Chem. **73**, 531 (1961).
[2]F. Steel and W. Birnkrant, Ber. **95**, 1264 (1962).

Components:

(1) Xenon fluoride; XeF_4; [13709-61-0]
(2) Nitrosyl fluoride; NOF; [7789-25-5]
(3) Hydrogen fluoride; HF; [7664-39-3]

Original Measurements:

N. S. Nikolaev, A. S. Nazarov, A. P. Opalovskii, and A. F. Trippel, Dokl. Acad. Nauk SSSR **186**, 1331–33 (1969).

Variables:

T/K=291.6–354.1

Prepared By:

Bruno Jasselskis

Experimental Values

Solubility of xenon tetrafluoride in a mixture of one mol NOF and three mol HF at 18.4 °C–80.9 °C

t/°C	T/K	XeF_4 solubility $100w_1$*	XeF_4 solubility (m_1/mol kg^{-1})
18.4	291.6	5.95, 6.87	0.33±0.04
40.2	313.4	10.45	0.56
60.0	333.2	15.38	0.88
80.9	354.1	21.22, 23.12	1.37±0.11

*The authors reported g solute per 100 g of solution and the compiler calculated the molal solubility values.

The solutions are nonconducting and stable. The enthalpy of solution (van't Hoff equation) is 20.5 kJ mol^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:

Solutions of appropriate concentration were prepared by weight in a dry box and hermetically sealed in teflon containers. Temperature was controlled to +0.2 °C. The saturated solutions were analyzed for nitrogen, fluorine and the amount of xenon tetrafluoride calculated.

Source and Purity of Materials:

(1) Xenon tetrafluoride. Reported purity of 98%.
(2) Nitrosyl fluoride.
(3) Hydrogen fluoride.
The NOF·3HF mixture prepared by the procedure of Steel and Birnkrant.[1,2] The NOF and excess anhydrous HF are mixed at 30 °C–40 °C. The solution is distilled and a fraction boiling at 94 °C–98 °C has the 1 mol NOF 3 mol HF composition. The conductivity is 2400 Ω^{-1} cm^{-1} (i.e., S/cm).

Estimated Error:

Not specified, but can be deduced from two values reported at 18.4 °C and 80.9 °C, the compiler estimates the reproducibility to be on the order of 10%–15%.

References:

[1]F. Steel and W. Birnkrant, Angew. Chem. **73**, 531 (1961).
[2]F. Steel and W. Birnkrant, Ber. **95**, 1264 (1962).

Components:
(1) Xenon fluoride; XeF_2; [13709-36-9]
(2) Iodine pentafluoride; IF_5; [7783-66-6]

Original Measurements:
A. V. Nikolaev, A. A. Opalovskii, A. S. Nazarov, and G. V. Tretyakov, Izv. Sib. Old. Akad. Nauk SSSR, Ser. Khim Nauk (No. 5), 21–27 (1972).

Variables:
T/K=288–343

Prepared By:
Bruno Jaselskis

Experimental Values

Solubility of XeF_2 in IF_5 from 15 °C to 70 °C

t/°C	T/K	XeF_2 solubility (m_1 /mol kg^{-1})
15	288	0.29
33	306	0.51
40	313	0.61
48	321	0.66
70	343	1.00

The estimated enthalpy of solution from the solubility data is (17±7) kJ mol^{-1}. The authors state the solubility varies with solvent as NOF>3HF>HF>IF_5.
No other information given.

Components:
(1) Xenon fluoride; XeF_4; [13709-61-0]
(2) Iodine pentafluoride; IF_5; [7783-66-6]

Original Measurements:
A. V. Nikolaev, A. A. Opalovskii, A. S Nazarov, and G. V. Tretyakov, Izv. Sib. Old Akad. Nauk SSSR, Ser. Khim Nauk (No. 5), 21–27 (1972).

Variables:
T/K=296.2–343.2

Prepared By:
Bruno Jaselskis

Experimental Values

Solubility of XeF_4 in IF_5 from 23 °C to 70 °C

t/°C	T/K	XeF_4 solubility (m_1 /mol kg^{-1})
23.0	296.2	0.74
30.0	303.2	0.99
36.2	309.2	1.19
44.0	317.2	1.26
55.0	328.2	1.43
70.0	343.2	1.74

The estimated enthalpy of solution from the solubility data ranges from 6 to 30 kJ mol^{-1}.
No other information given.

Components:
(1) Xenon fluoride; XeF_2; [13709-36-9]
(2) Acetonitrile; CH_3CN; [75-05-8]

Original Measurements:
H. Meinet and St. Rudinger, Z. Chem. **7**, 239–240 (1967).

Variables:
T/K = 273, 294

Prepared By:
Bruno Jaselskis

Experimental Values

t/°C	T/K	XeF_2 solubility (ρ_1 /g L^{-1})	XeF_2 solubility (c_1 /mol L^{-1})
0	273	168	0.99
21	294	210	1.34

The compiler calculated the solubilities in mol L^{-1}.

The solutions are nonionic and the enthalpy of solution was estimated to be 7.2 kJ mol^{-1}. At −10 °C solutions of XeF_2 in pure acetonitrile are stable for long periods of time. At room temperature they decompose in about 24 days. In the presence of water in the acetonitrile, XeF_2 decomposes to form HF which catalyses further decomposition.

Components:
(1) Xenon fluoride; XeF_2; [13709-36-9]
(2) Uranium hexafluoride; UF_6; [7783-81-5]

Original Measurements:
N. S. Nikolaev and A. T. Sadikova, Atom. Energia **39**, 339–443 (1975); Sov. At. Energy (Engl. transl.) **39**, 982–87 (1975).

Variables:
T/K = 373

Prepared By:
Bruno Jaselskis

Experimental Values

The solubility of XeF_2 in UF_6 at 100 ± 5 °C is 167 g XeF_2 per kg of UF_6 [m_1 = 1.18 mol kg^{-1} (compiler)].

The measurement was carried out in a copper autoclave.

3.2. Trifluoroborane

Components:
(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Aromatic hydrocarbons
(3) Hydrofluoric acid; HF; [7664-39-3]

Evaluators:
H. Lawrence Clever,
Emory University,
Atlanta, GA 30322
April 2003

Evaluation

Part I. Trifluoroborane+Hydrogen fluoride

The solubility of trifluoroborane, BF_3, in anhydrous hydrofluoric acid has been reported in five papers. The available data are summarized in Table 3.

References 3, 4, and 5 present their data in figures. References 4 and 5 fit their data to equations. The equations and figures are on the respective data sheets. There is no data sheet for Ref. 3. The mole fraction solubility at a partial pressure of 0.1013 MPa from the first four references falls near the same $\ln x_1$ vs $1/(T/K)$ line. The data from Ref. 5 is definitely of larger value than the other data. This may be misleading. The authors[5] measured to a much larger pressure and fitted the data to straight lines that did not go to the origin. This causes the 0.1013 MPa data to be too large. If we had the authors numerical data the data could be refitted with equations that are forced through the origin and better low pressure solubility values could be obtained. Also, any departure from Henry's law would be more apparent. See the figure on Ref. 4 data sheet. The Evaluator believes it likely that the high-pressure data from Ref. 5 may be reliable for many purposes. He also suggests that the 0.1013 MPa solubility data from Ref. 2, which covers the temperature interval of 199.2–316.5 K, be used as a self consistent data set. All of the data are classed as tentative.

Part 2. Trifluoroborane+Aromatic Hydrocarbons+Aromatic Hydrocarbons+Hydrofluoric acid

References 1, 3, and 5 contain data on the three component systems. The data from Ref. 1 on 1,2-dimethylbenzene, 1,3-dimethylbenzene and 1,4-dimethylbenzene is on a data sheet. These data are reproduced on a graph in Ref. 3 along with data on methylbenzene, 1,3,5-trimethylbenzene, and hexamethylbenzene. Since the data on the last three systems are only on a graph they have not been reproduced here.

The methylbenzenes show increasing basicity as the number of methyl groups on the benzene ring increases. In the BF_3+Ar+HF the reaction: $Ar+HF+BF_3=[ArH]^+ + BF_4^-$ is postulated. The vapor pressure experiments described here and batch extraction experiments were analyzed by the authors[1,3] to obtain the relative basicity of the methyl substituted benzenes with respect to reaction with the $HF+BF_3$.

The relative basicity is given in the following table. The 1,4-dimethylbenzene is the first member in the series to show appreciable basicity toward $HF+BF_3$. The value for methylbenzene was estimated from vapor pressure measurements. Benzene is too weak a base for a determination of its relative basicity by this method.

Relative basicity of aromatic hydrocarbons.

Aromatic Hydrocarbon	Basicity Relative to 1,4-Dimethylbenzene as the Standard
Methylbenzene	(~0.01)
1,4-Dimethylbenzene	1
1,2-Dimethylbenzene	3
1,3-Dimethylbenzene	9
1,2,4-Trimethylbenzene	18
1,2,3-Trimethylbenzene	(~18)
1,3,4,5-Tetramethylbenzene	60
1,2,3,4-Tetramethylbenzene	85
1,3,5-Trimethylbenzene	1400
1,2,3,5-Tetramethylbenzene	2800
Pentamethylbenzene	4350
Hexamethylbenzene	44500

All of the solubility data (vapor pressure) for these systems from McCauley *et al.*[1] and McCauley and Lien[3] are classed as tentative.

References

[1]D. A. McCaulay, B. H. Shoemaker, and A. P. Lien, Ind. Eng. Chem. **42**, 2103–2107 (1950).
[2]E. C. Hughes and S. M. Darling, Ind. Eng. Chem. **43**, 746–750 (1951).
[3]D. A. McCaulay and A. P. Lien, J. Am. Chem. Soc. **73**, 2013 (1951).
[4]M. Kilpatrick and F. E. Luborsky, J. Am. Chem. Soc. **76**, 5865–5868 (1954).
[5]R. J. Mikovsky, S. D. Levy, and A. L. Hensley Jr., J. Chem. Eng. Data **6**, 603–604 (1961).

TABLE 3. Comparison of solubility of BF_3 in HF from five papers

Temperature (T/K)	Partial pressure (p_1/MPa)	Mole fraction at 0.1013 MPa x_1	Reference
199.2	0.1013	0.0746	2
230.2	0.1013	0.0496	2
242.2	0.1013	0.0376	2
247.2	0.1013	0.0329	2
273.2	0–0.184	0.013	1, 3
277.6	0.1013–1.240	0.0064	2
292.4	0.1013–0.709	0.0028	4
293.7	0.1013–1.240	0.0051	2
297.2	0–6.90	0.0125	5
316.5	0.1013–1.240	0.0034	2
322.2	0–6.90	0.0095	5
371.2	0–6.90	0.0034	5

Components:
(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Hydrofluoric acid; HF; [7664-39-3]

Original Measurements:
D. A. McCaulay, B. H. Shoemaker, and A. P. Lien, Ind. Eng. Chem. **42**, 2103-07 (1950).

Variables:
T/K = 273.15
p_1 /MPa = 0 – 0.184

Prepared By:
H. L. Clever

Experimental Values

Vapor pressure of the BF_3 + HF system at 0 °C

BF_3/	HF/g	p_{tot} /cm Hg	p_1 /cm Hg	p_1 /MPa	BF_3 /g	x_1
0	106	38	0	0.0	0	0
3.5	106	67	29	0.039	2.8	0.008
7.0	106	122	84	0.112	5.0	0.014
10.5	106	176	138	0.184	7.2	0.020

The compiler added the BF_3 partial pressures in MPa.
The equilibrium mixtures were contained in a 600 mL copper flask. The first two columns given the initial composition of the system, the last two columns give the BF_3 in solution at equilibrium.

Auxiliary Information

Method/Apparatus/Procedure:
The vapor pressure apparatus consisted of a 600 mL copper flask for the equilibrium mixture, a copper helix connection to allow agitation, a 1200 mL copper flask for metering the BF_3, a BF_3 storage cylinder and a 30 lb in.$^{-2}$ pressure gage. All were attached to a 0.6 in. copper manifold and vacuum line. Valves were Teflon packed Hoke needle valves.
A weighed amount of HF was added to the equilibrium flask, it was frozen in liquid nitrogen and evacuated. BF_3 was transferred to the metering flask at a known pressure, then condensed into the equilibrium flask. The equilibrium vessel was brought to 0 °C, agitated by hand until the pressure was constant (about 1–2 h). The contents were again frozen in liquid nitrogen, evacuated and more BF_3 added and the procedure repeated.

Source and Purity of Materials:
(1) Boron trifluoride. Harshaw Chemical Co. 96% purity, the 4% impurity was an inert noncondensable gas which was removed by evacuation from the frozen BF_3.
(2) Hydrogen fluoride. Harshaw Chemical Co. 99.6% purity.

Estimated Error:
Temperature and pressure. Nothing specified.
$\delta x_1 / x_1 = 0.05$ (Compiler).
These data are given graphically in a later paper.[1]

References:
[1]D. A. McCaulay and A. P. Lien, J. Am. Chem. Soc. **73**, 2013 (1951).

Components:
(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Hydrofluoric acid; HF; [7664-39-3]

Original Measurements:
E. C. Hughes and S. M. Darling, Ind. Eng. Chem. **43**, 746–750 (1951).

Variables:
T/K = 199.2 – 316.4
p_1 /MPa = 0.1013 – 1.240

Prepared By:
H. L. Clever

Experimental Values

Temperature		Pressure		BF_3 solubility
(t/°C)	(T/K)	(p_1 /lb in.$^{-2}$)	(p_1 /MPa)	x_1
74	199.2	14.7	0.1013	0.0746
−43	230.2	14.7	0.1013	0.0496
−31	242.2	14.7	0.1013	0.0376
−26	247.2	14.7	0.1013	0.0329
4.4	277.6	14.7	0.1013	0.0064
4.4	277.6	60	0.4135	0.0225
4.4	277.6	120	0.8269	0.0420
4.4	277.6	180	1.2404	0.0618
20.5	293.7	14.7	0.1013	0.0051
20.5	293.7	60	0.4135	0.0192
20.5	293.7	120	0.8269	0.0335
20.5	293.7	180	1.2404	0.0477
43.3	316.5	14.7	0.1013	0.0034
43.3	316.5	60	0.4135	0.0118
43.3	316.5	120	0.8269	0.0221
43.3	316.5	180	1.2404	0.0322

The compiler changed the author's values from mol % to mole fraction and added the Kelvin temperatures and the MPa pressures.

Auxiliary Information

Method/Apparatus/Procedure:
The authors present a table of solubility values, but do not give details of the method or discuss their solubility results. Their experiments on the thermal reforming of lower paraffin hydrocarbons were carried out in Monel metal vessels with copper transfer lines. It is assumed the apparatus was used in the solubility measurements.
The authors describe a measurement of the mutual solubility of HF and BF_3 in a dearomatized Pennsylvania kerosene as 0.451 wt % HF and 0.251 wt % BF_3 at 26 °C (299 K) and 150 lb in.$^{-2}$ (1034 MPa) gage pressure.

Source and Purity of Materials:
(1) Boron trifluoride. Harshaw Chemical Co. Used as received.
(2) Hydrogen fluoride. Harshaw Chemical Co. Obtained in cylinder form and used as received.

Estimated Error:
No estimate possible.

Components:

(1) Triborane; BF_3; [7637-07-2]
(2) Hydrofluoric acid; HF; [7664-39-3]

Original Measurements:

M. Kilpatrick and F. E. Luborsky, J. Am. Chem. Soc. **79**, 5865–5868 (1954).

Variables:

T/K=292.4
p_{tot}/kPa=101.3–709.1

Prepared By:

H. L. Clever

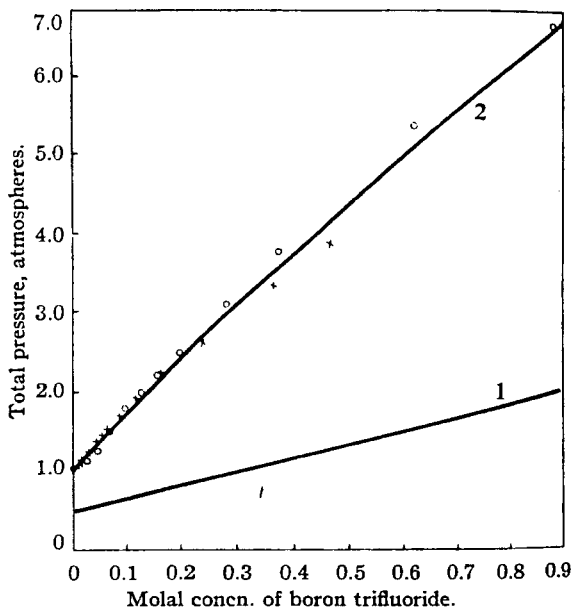
Experimental Values

The data are presented in a graph of total pressure vs boron trifluoride molality (see figure below). The author's data are linear to a total pressure of 2.5 atm. The linear part of the curve follows the equation:

$$p_{tot}/\text{atm}=7.17(m_1/\text{mol kg}^{-1})+1.0.$$

The compiler calculated the BF_3 solubility (molality) at 19.2 °C (292.4 K) as a function of total pressure in anhydrous HF from the above equation.

P_{tot}/atm	p_1/atm	m_1/mol kg^{-1}
1.0	0.0	0.0
1.5	0.5	0.070
2.0	1.0	0.14
2.5	1.5	0.21



—Solubility of BF_3 in HF: 1, McCaulay and Lien at 0°; this investigation at 19°.

Curve 1 in the figure at 0 °C is from D. A. McCauly and A. R. Lien, J. Am. Chem. Soc. **73**, 2013 (1951). It was apparently estimated by the present authors from a figure in the paper. Curve 2 is the author's data at 19.4 °C.

Auxiliary Information

Method/Apparatus/Procedure:

The boron trifluoride dissolved in the hydrofluoric acid was calculated from the difference between the total BF_3 gas added to the vapor phase above the solution and the BF_3 gas remaining in the vapor phase above the solution after equilibrium was established. The BF_3 remaining in the vapor phase was calculated from the measured volumes of the cell and the liquid assuming Dalton's law.
At low pressure the total pressure of the system was found to be a linear function of the BF_3 molality in solution. The deviation from linearity at higher pressures can be attributed to the compressibility of the gas and/or deviations from Dalton's law.

Source and Purity of Materials:

(1) Boron trifluoride. Harshaw Chemical Co. Purified by forming the benzene nitrile addition compound, purified under vacuum, then thermal decomposition at low temperature.[1]
(2) Hydrofluoric acid. Technical grade KHF_2 dried and thermally decomposed to form HF, which was distilled. The final HF product contained less than 0.0005 mol kg^{-1} of water.

Estimated Error:

$\delta m_1/m_1=\pm 0.05$ (Compiler estimated).

References:

[1]M. Kilpatrick and F. E. Luborsky, J. Am. Chem. Soc. **75**, 577 (1953).

Components:

(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Hydrofluoric acid; HF; [7664-39-3]

Original Measurements:

R. J. Mikovsky, S. D. Levy, and A. L. Hensley Jr., J. Chem. Eng. Data **6**, 603–604 (1961).

Variables:

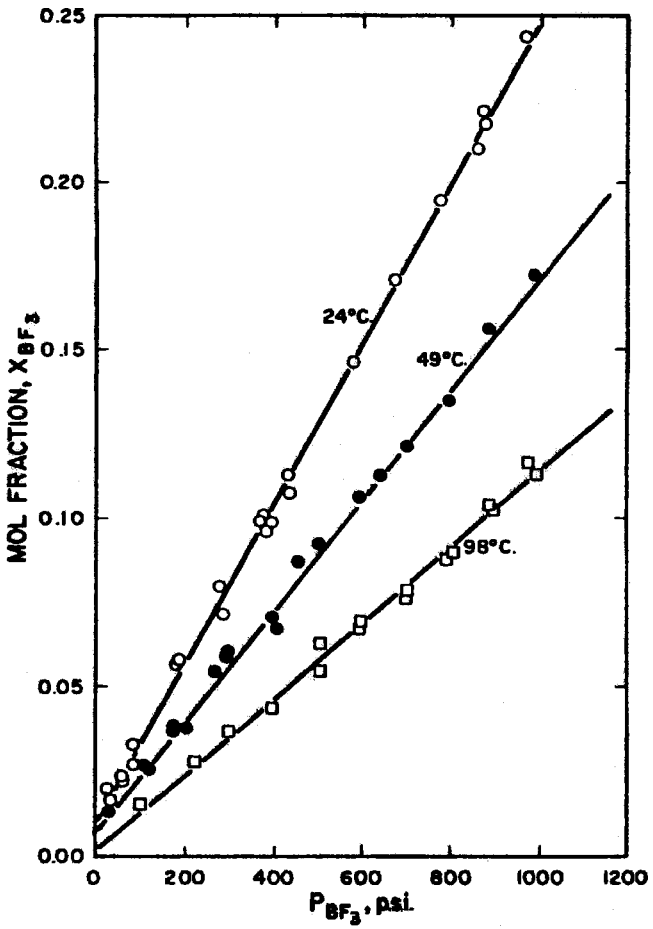
T/K=297.2, 322.2, and 371.2
p_1 /MPa=0–6.90

Prepared By:

H. L. Clever

Experimental Values

Measurements were made at temperatures of 24, 49, and 98 °C and BF_3 partial pressures between 0 and 1000 lb in.$^{-2}$. The results are presented in a large-scale graph, which is reproduced below. The BF_3 mole fraction increases linearly with the BF_3 partial pressure. The author's least square lines do not go exactly to the origin. Equations for the least square lines are given.



At 24 °C (297.2 K). $x_1=(9.07\times10^{-3})+(2.36\times10^{-4})(p_1$ /lb in$^{-2})$ At 49 °C (322.2 K). $x_1=(7.02\times10^{-3})+(1.70\times10^{-4})\times(p_1$ /lb in$^{-2})$
At 98 °C (371.2 K). $x_1=(1.77\times10^{-3})+(1.11\times10^{-4})(p_1$ /lb in$^{-2})$
In the equations above x_1 is BF_3 mol fraction; p_1 BF_3 partial pressure in lb in.$^{-2}$

Auxiliary Information

Method/Apparatus/Procedure:

To a closed Hastalloy-B autoclave was added about 200 mL HF; HF vapor pressure measured. BF_3 added and mixture stirred 20–30 m. The total pressure measured and equilibrium p of BF_3 obtained by difference (p_t-p_{HF}). The equilibrium liquid phase sampled through a metering valve in bottom. BF_3 analyzed by hydrolysis in presence of Ca^{2+} then titration with strong acid to form H_3BO_3.

Source and Purity of Materials:

(1) Boron trifluoride. Source not given. Stated to be 99.0% minimum purity.
(2) Hydrogen fluoride. Source not given. Stated to be 99.9% minimum purity.

Estimated Error:

$\delta x_1/x_1=\pm0.03$ (Compiler estimate).

Components:
(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Nitrogen oxide; NO; [10102-43-9]

Original Measurements:
V. Ribnikar, Z. Pupezin, Z. Knezevic, E. Cuker, and V. Dokic, Abhandl, Deut. Akad. Wiss. Berlin Kl. Chem. Geol. Biol. (**7**), 155–161 (1963) (Publ. 1965).

Variables:
Liquid air temperatures (undefined).

Prepared By:
H. L. Clever

Experimental Values

Observations on the BF_3+NO system at liquid air temperatures and above.

When a mixture of NO and BF_3 gases is cooled to liquid air temperatures, an orange colored solid is formed. The solid melts to a purple-red liquid at 143 K and the liquid stays colored until 163 K. A simple distillation of the material condensed from 1:1 gas mixtures at pressures between 150 and 760 Torr gave back the component gases. The colored solids, probably $NO{\cdot}BF_3$ accompanied with a white solid which also forms in the mixture. It was found to be $NO_2{\cdot}BF_3$. The author suggests the disproportionation reaction

$$3NO = NO_2 + N_2O$$

is probably induced by the liquid BF_3 at low temperature.

Auxiliary Information

Method/Apparatus/Procedure:
Nothing specified.

Source and Purity of Material:
Nothing specified for either component.

Estimated Error:
Nothing specified.

Components:
(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Pentane; C_5H_{12}; [109-66-0]

Original Measurements:
G. N. Cade, R. E. Dunn, and H. J. Hepp, J. Am. Chem. Soc. **68**, 2454–55 (1946).

Variables:
T/K = 322.2, 339.2, and 366.2
p_{tot}/MPa = 0.385– 1.50

Prepared By:
H. L. Clever

Experimental Values

Temperature*		Pressure*		Composition Vapor Phase		Composition Liq Phase	
(t/°C)	(T/K)	(p_{tot}/atm)	(p_{tot}/MPa)	10^2x_1	10^2x_2	10^2x_1	10^2x_2
49	322.2	4.0	0.405	61.9	38.1	0.55	99.45
49	322.2	6.7	0.679	75.9	24.1	1.27	98.73
49	322.2	9.2	0.932	80.5	19.5	1.88	98.12
49	322.2	11.9	1.206	83.9	16.1	2.89	97.11
49	322.2	14.7	1.489	84.5	15.5	3.64	96.36
66	339.2	3.8	0.385	37.9	62.1	0.24	99.76
66	339.2	6.5	0.659	67.1	32.9	0.86	99.14
66	339.2	9.2	0.932	76.2	23.8	1.53	98.47
66	339.2	11.9	1.206	77.8	22.2	2.16	97.84
66	339.2	14.8	1.500	82.7	17.3	3.12	96.88
93	366.2	6.5	0.628	22.7	77.3	44.4	99.73
93	366.2	8.9	0.902	42.8	77.3	0.86	99.14
93	366.2	9.1	0.922	49.6	50.4	1.06	98.94
93	366.2	12.2	1.236	—	---	1.91	98.09
93	366.2	12.4	2.256	55.6	44.4	2.00	98.00

*The compiler calculated and added the Kelvin temperatures and the pressures in MPa.

The authors calculated the mL (STP) of BF_3 per g of pentane and plotted the values against the total pressure. The solubility in this unit (Kuenen coefficient) ranged from about 1 to 12 and the graphs were slightly concave upwards. Isobars at 3.0, 4.0, 5.0, 6.0, and 7.0 atm partial pressure BF_3 show a minimum solubility at about 70 °C (343 K).

Auxiliary Information

Method/Apparatus/Procedure:
About 3 L of pentane was charged to an evacuated 7.5 L copper platted steel reactor vessel equipped with a motor driven stirrer, a calibrated Bourdon-tube pressure gage, a thermometer well and sample outlets for liquid and vapor phases. The reactor vessel and contents were brought to temperature in a thermostated water or oil bath, BF_3 was forced into the reactor to the desired pressure. The reactor vessel was stirred for 8–12 h, a constant pressure for 4 h was taken as evidence equilibrium was reached. Vapor and liquid samples were taken in 5 and 25 mL stainless steel containers equipped with brass Hoke needle valves. The samples were vaporized, diluted with dry N_2, and passed through a tarred Ascarite tube. The BF_3 was absorbed by the Ascarite and determined by the weight increase.

Source and Purity of Materials:
(1) Boron trifluoride. Harshaw Chemical Co. Used as received.
(2) Pentane. Phillips Petroleum Co. Dried by distillation and used without further purification. The author's analysis after the experiment gave 99.7% pentane and 0.3% isopentane.

Estimated Error:
δT/K = ±0.5 (authors).
$\delta S/S$ = ±0.05 (authors).

Components:
(1) Trifluoroborane; BF_3; [7637-07-3]
(2) Aromatic hydrocarbons

Evaluator:
H. Lawrence Clever,
Emory University,
Atlanta, GA 30322
2002

Evaluation

Some comments on the solubility of trifluoroborane in aromatic hydrocarbons.

Two laboratories report values of the solubility trifluoroborane, BF_3, in various aromatic hydrocarbons. Wheeler and Keating[1] report values of the BF_3 solubility in benzene and in methylbenzne at 0.101325 MPa partial pressure between temperatures of 295 K and 320 K. Kozarezov, Rusakov, Pikalo, and Lazareva[2] report values of the BF_3 solubility in benzene, ethylbenzene, and diethylbenzene at pressures between 0.152 and 0.768 MPa over the temperature interval of 293–373 K.

Only the $BF_3+C_6H_6$ system was measured by both laboratories. Unfortunately the agreement between the two groups of workers is poor leaving in doubt the other systems they measured. In Table 4 we compare results of the two groups. The KRPL[2] data were reduced to 0.101325 MPa (1 atm) using and assuming the validity of Henry's law.

The KRPL[2] Bunsen coefficients were calculated from their Kuenen coefficients, not the mole fractions, which accounts for the different trends. Most of their mole fractions were given to only one significant digit.

The laboratory's results differ by about 25%. We cannot make a choice as to which is the more reliable. We class both results as tentative, and advise use with caution.

References

C. M. Wheeler and H. P. Keating, J. Phys. Chem. **58**, 1171–1172 (1954).
Yu. I. Kozarezov, A. P. Rusakov, N. M. Pikalo, and O. A. Lazareva, Zh. Fiz. Khim. **45**, 2373 (1971); Dep. Doc. VINITI N3047-71 (21/06/71).

TABLE 4. Comparison of results of two laboratory results for the $BF_3+C_6H_6$ system

Laboratory	T/K	Solubility at 0.101325 MPa 10^3x_1	Bunsen Coefficient at 0.101325 MPa (α/cm^3 cm^{-3} atm^{-1})
WK[1]	295	2.47	0.620
WK[1]	320	2.26	0.543
KRPL[2]	293	1.5	0.39
KRPL[2]	293	1.8	0.45
KRPL[2]	293	1.7	0.45
KRPL[2]	323	1.6	0.36
KRPL[2]		1.4	0.36
		1.5	0.36
		1.5	0.40

Components:
(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:
C. M. Wheeler and H. P. Keating, J. Phys. Chem. 58, 171–72 (1954).

Variables:
T/K = 295–320
p_1 /kPa = 101.3 (1 atm)

Prepared By:
H. L. Clever

Experimental Values

T/K	Mole Fraction 10^3x_1	Bunsen Coefficient (α/cm^3 cm^{-3} atm^{-1})	Ostwald Coefficient (L/cm^3 cm^{-3})
295	2.47	0.620	0.670
300	2.42	0.602	0.662
305	2.39	2.26	0.658
310	2.36	0.572	0.650
315	2.29	0.559	0.645
320	2.26	0.543	0.636

The compiler calculated the Bunsen coefficients from the authors Ostwald values assuming ideal gas behavior.

The authors fitted the mole fraction solubilities to the van't Hoff equation to obtain the thermodynamic changes:

$$\Delta H^\circ = -2.890 \text{ kJ mol}^{-1} \text{ and } \Delta S^\circ = -62.6 \text{ J K}^{-1} \text{ mol}^{-1}.$$

Auxiliary Information

Method/Apparatus/Procedure:
A modified Lannung[1] apparatus was used. It was modified so gas could be directly introduced from the gas cylinder to the apparatus, and mercury was used to prevent contact between either gas or solvent with stopcock grease. The solvent was degassed by refluxing.
The solvent volume was about 20 mL and the initial gas volume between 30 and 35 mL in all experiments. The gas burette could be read to 0.05 mL. The entire apparatus was thermostated by circulating water through a water jacket

Source and Purity of Materials:
(1) Boron trifluoride. Matheson Chemical Co. Reagent grade. Used as received.
(2) Benzene. Mallinckrodt Analytical Reagent. Dried over Na wire and distilled in a Todd column. R. I n^{25}_D=1.4979.

Estimated Error:
δT/K = ⇑0.05
$\delta x_1 / x_1 = \pm 0.03$ (compiler).

References:
[1]A. Lannung, J. Am. Chem. Soc. **52**, 68 (1930).

Components:
(1) Trifluoroborane; BF_3; [7637-07-3]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:
Yu. I. Kozarezov, A. P. Rusakov, N. M. Pikalo, and O. A. Lazareva, Zh. Fiz. Khim. **45**, 2373 (1971); Dep. Doc. VINITI N3047-71 (21/06/71).

Variables:
T/K = 293–373
p_1 /MPa = 0.14–0.95

Prepared By:
Yu. P. Yampol'skii

Experimental Values

Solubility of BF_3 in benzene at 20, 50, 75, and 100 °C at pressures between 1.40 atm and 9.34 atm

Temperature		Pressure		Solubility	
(T/K)	(t/°C)	(p_1 /atm)	(p_1 /Mpa)	x_1	Kuenen Coefficient [S/cm^3 (STP) g^{-1}]
20	293	2.60	0.263	0.004	1.16
20	293	5.10	0.525	0.009	2.59
20	293	7.60	0.778	0.013	3.93
250	323	1.87	0.189	0.003	0.78
250	323	2.87	0.291	0.004	1.19
250	323	5.37	0.544	0.008	2.42
250	323	7.87	0.797	0.012	3.58
75	348	1.40	0.142	0.001	0.24
75	348	3.40	0.353	0.004	1.19
75	348	5.90	0.606	0.007	2.13
75	348	8.40	0.851	0.011	3.20
100	373	3.34	0.338	0.002	0.62
100	373	4.34	0.440	0.004	1.05
100	373	6.84	0.693	0.007	2.05
100	373	9.34	0.946	0.011	3.12

Henry Constants: 20 °C, 580; 50 °C, 591; 75 °C, 650; 100 °C, 698 atm.
$\log(K/\text{atm}) = 3.100 - 100/(T/\text{K})$; $(K/\text{atm}) = (p/\text{atm})x_1$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by a manometric method.

Source and Purity of Materials:
(1) Boron trifluoride. Source not given. Purity stated to be 99.63%.
(2) Benzene. Source not given. Properties. Sp. Gr. d^{20}_4 = 0.8796; n^{20}_D = 1.5010, t_{cryst} = +5.4 °C; t_{bp} = 80 °C and water content 0.0015%.

Estimated Error:
Nothing specified. Compiler estimates 3%–10% reproducibility.

Components:
(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Methylbenzene; C_7H_8; [108-88-3]

Original Measurements:
C. M. Wheeler and H. P. Keating, J. Phys. Chem. **58**, 1171–72 (1954).

Variables:
T/K = 295–320
p_1 /kPa = 101.3 (1 atm)

Prepared By:
H. L. Clever

Experimental Values*

	Mole Fraction	Bunsen Coefficient	Ostwald Coefficient
T/K	$10^3 x_1$	(α/cm^3 cm^{-3} atm^{-1})	(L/cm^3 cm^{-3})
295	2.79	0.573	0.630
304	2.74	0.561	0.635
310	2.68	0.544	0.618
312	2.66	0.538	0.615
316	2.66	0.528	0.611
322	2.54	0.511	0.603

*The compiler calculated the Bunsen coefficients from the authors' Ostwald values assuming ideal gas behavior.

The authors fitted the mole fraction solubilities to the van't Hoff equation to obtain the thermodynamic changes:

$$\Delta H° = -3.314 \text{ kJ mol}^{-1} \text{ and } \Delta S° = -62.6 \text{ J K}^{1} \text{ mol}^{-1}.$$

Auxiliary Information

Method/Apparatus/Procedure:
A modified Lannung[1] apparatus was used. It was modified so gas could be directly introduced from the gas cylinder to the apparatus, and mercury was used to prevent contact between either gas or solvent with stopcock grease. The solvent was degassed by refluxing.
The solvent volume was about 20 mL and the initial gas volume between 30 and 35 mL in all experiments. The gas burette could be read to 0.05 mL. The entire apparatus was thermostated by circulating water through a water jacket.

Source and Purity of Materials:
(1) Boron trifluoride. Matheson Chemical Co. Reagent grade. Used as received.
(2) Methyl benzene (toluene). Merck Reagent Grade. Dried over Na wire and distilled in a Todd column. R. I. n^{25}_D = 1.4939.

Estimated Error:
δT/K = ±0.05.
$\delta x_1 / x_1$ = ±0.03 (compiler).

References:
[1]A. Lannung, J. Am. Chem. Soc. **52**, 68 (1930).

Components:

(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Dimethylbenzenes; C_8H_{10}. See below.
(3) Hydrofluoric acid; HF; [7664-39-3]

Original Measurements:

D. A. McCaulay, B. H. Shoemaker, and A. P. Lien, Ind. Eng. Chem. **42**, 2103–07 (1950).

Variables:

T/K=273.15
p_1 /MPa=0–0.223

Prepared By:

H. L. Clever

Experimental Values

Vapor pressure for $BF_3+C_8H_{10}+HF$ at 273.15 K for 1,2-Dimethylbenzene (*o*-xylene); C_8H_{10}; [95-47-6]

Initial Masses			Equilibrium Pressure			BF_3 in solution	
BF_3	C_8H_{10} /g	HF/g	(p_{tot} /cmHg)	(p_1 /cmHg)	(p_1 /MPa)	(g_1 /g)	x_1
0	44	99.5	36	0	0	0	0
12.5	44	99.5	62	27	0.036	12.1	0.036
25.0	44	99.5	117	84	0.112	23.5	0.070
33.3	44	99.5	171	138	0.184	30.3	0.090
37.5	44	99.5	199	167	0.223	34.4	0.102

Vapor pressure for $BF_3+C_8H_{10}+HF$ at 273.15 K for 1,3-Dimethylbenzene (*m*-xylene); C_8H_{10}; [108-38-3].

Initial Masses			Equilibrium Pressure			BF_3 in solution	
BF_3	C_8H_{10} /g	HF/g	(p_{tot} /cmHg)	(p_1 /cmHg)	(p_1 /MPa)	g_1 /g	x_1
0	44	93.5	36	0	0	0	0
10.7	44	93.5	42	6	0.008	10.6	0.033
21.3	44	93.5	39	3	0.004	21.2	0.067
28.4	44	93.5	75	42	0.056	27.5	0.086
32.0	44	93.5	100	68	0.091	30.3	0.095
33.5	44	93.5	129	97	0.129	32.2	0.102

Vapor pressure for $BF_3+C_8H_{10}+HF$ at 273.15 K for 1,4-Dimethylbenzene (*p*-xylene); C_8H_{10}; [106-42-3].

Initial Masses			Equilibrium Pressure			BF_3 in solution	
BF_3	C_8H_{10} /g	HF/g	(p_{tot} /cmHg)	(p_1 /cmHg)	(p_1 /MPa)	g_1 /g	x_1
0	41	109.5	36	0	0	0	0
10.7	41	109.5	67	32	0.043	10.0	0.027
21.4	41	109.5	92	92	0.123	19.4	0.052
28.5	41	109.5	139	139	0.185	25.4	0.068

The compiler added the BF_3 partial pressures in MPa.

Auxiliary Information

Method/Apparatus/Procedure:

The vapor pressure apparatus consisted of a 600 mL copper flask for the equilibrium mixture connected through a copper tube helix to allow agitation, a 1200 mL copper flask for metering the BF_3, a BF_3 storage cylinder and a 30 lb in.$^{-2}$ pressure gage. All components were attached to a 0.6 in. copper manifold and vacuum line. Valves were Teflon packed Hoke needle valves.

Weighed amounts of HF and C_8H_{10} were added to the equilibrium flask, it was frozen in liquid nitrogen and evacuated. BF_3 was transferred to the metering flask at a known pressure, then condensed into the equilibrium flask. The equilibrium flask was brought to 0 °C, agitated by hand until the pressure was constant (about 1–2 h). The contents were again frozen in liquid nitrogen, evacuated and more BF_3 added and the procedure repeated.

Source and Purity of Materials:

(1) Boron trifluoride. Harshaw Chemical Co. Purity 96%, the 4% impurity was an inert, noncondensable gas which was removed by evacuation from the frozen BF_3.
(2) Xylenes. Eastman Kodak Co. No further information.
(3) Hydrofluoric acid. Harshaw Chemical Co. Purity 99.6%. Used as received.
These and additional data are presented in graphs in a later paper.[1]

References:

D. A. McCaulay and A. P. Lien, J. Am. Chem. Soc. **73**, 2013 (1951).

Components:
(1) Trifluoroborane; BF_3; [7637-07-3]
(2) Ethylbenzene; C_8H_{10}; [100-41-4]

Original Measurements:
Yu. I. Kozorezov, A. P. Rusakov, N. M. Pikalo, and O. A. Lazareva, Zh. Fiz. Khim. **45**, 2373 (1971); Dep. Doc. VINITI N3047-71 (21/06/71)

Variables:
T/K = 293–423
p_1 /MPa = 0.15–0.91

Prepared By:
Yu. P. Yampol'skii

Experimental Values

Solubility of BF_3 in ethylbenzene at 20 °C, 50 °C, 100 °C, and 150 °C at pressures between 1.55 and 9.00 atm

Temperature		Pressure		Solubility	
(t/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	x_1	Kuenen Coefficient [S/cm^3 (STP) g^{-1}]
20	293	2.51	0.254	0.005	1.14
20	293	5.01	0.508	0.010	2.23
20	293	7.51	0.761	0.016	3.42
50	323	1.55	0.157	0.003	0.66
50	323	2.55	0.258	0.005	1.04
50	323	5.05	0.512	0.009	1.93
50	323	7.55	0.765	0.013	2.89
100	373	1.85	0.187	0.002	0.51
100	373	2.85	0.289	0.004	0.92
100	373	5.35	0.542	0.008	1.65
100	373	7.85	0.795	0.012	2.52
150	423	3.00	0.304	0.002	0.46
150	423	4.00	0.405	0.004	0.75
150	423	6.50	0.659	0.007	1.59
150	423	9.00	0.912	0.011	2.35

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by a manometric method.

Source and Purity of Materials:
(1) Boron trifluoride. Source not given. Purity stated to be 99.63%.
(2) Ethylbenzene. Source not given. Properties. Sp. Gr. d^{20}_4 = 0.8673; n^{20}_D = 1.4960, t_{bp} = 80 °C and water content 0.0028%.

Estimated Error:
Nothing specified. Compiler estimates a reproducibility of around 3%–10%.

Components:
(1) Trifluoroborane; BF_3; [7637-07-3]
(2) Diethylbenzene; $C_{10}H_{14}$; [25340-17-4]

Original Measurements:
Yu. I. Kozorezov, A. P. Rusakov, N. M. Pikalo, and O. A. Lazareva, Zh. Fiz. Khim. **45**, 2373 (1971); Dep. Doc. VINITI N3047-71 (21/06/71).

Variables:
T/K = 293–373
p_1 /MPa = 0.15–0.77

Prepared By:
Yu. P. Yampol'skii

Experimental Values

Solubility of BF_3 in diethylbenzene at 20 °C, 50 °C, and 100 °C at pressures between 1.0 atm and 7.68 atm

Temperature		Pressure		Solubility	
(t/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	x_1	Kuenen Coefficient (S/cm^3 (STP) g^{-1})
20	293	1.50	0.152	0.003	0.57
20	293	2.50	0.253	0.006	0.98
20	293	5.00	0.507	0.012	2.04
20	293	7.50	0.760	0.018	3.00
50	323	1.51	0.153	0.003	0.50
50	323	2.51	0.254	0.004	0.74
50	323	5.01	0.508	0.009	1.45
50	323	7.51	0.761	0.013	2.21
100	373	1.58	0.160	0.002	0.40
100	373	2.58	0.261	0.004	0.64
100	373	5.08	0.515	0.007	1.24
100	373	7.58	0.768	0.011	1.86

Henry Constants: 20 °C, 426; 50 °C, 558; 100 °C, 655
$(K/\text{atm}) = (p_1/\text{atm})x_1$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by a manometric method.

Estimated Error:
Nothing specified. Compiler estimates a reproducibility of around 3%–10%.

Components:

(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

Original Measurements:

H. C. Brown and R. R. Holmes, J. Am. Chem. Soc. **78**, 2173–76 (1956).

Variables:

T/K=278.40–297.25

Prepared By:

H. L. Clever

Experimental Values

Henry's constants for BF_3 in nitrobenzene at temperatures from 5.25 °C to 24.10 °C

Temperature (t/°C)	Temperature (T/K)	Henry's constant (10^{-3} k/mmHg)
Series 1		
5.68	278.83	6.51
14.50	287.65	11.1
24.10	297.25	18.3
Series 2		
5.25	278.40	6.25
15.03	278.40	11.2
24.10	297.25	18.1

The Henry's Constant: k/mmHg=(p_1 /mmHg)/x_1.

The authors show log (k/mmHg) vs 1/(T/K) is linear. The enthalpy of solution of BF_3 in nitrobenzene is: $\Delta H°=-(9.24 \pm 0.12)$ kcal mol^{-1} $-(38.66 \pm 0.50)$ kJ mol^{-1} (Compiler).

Auxiliary Information

Method/Apparatus/Procedure:

No experimental details are given. The pressure range was not stated.
It is likely the same procedure and apparatus were used in this work as in Brown's earlier work on the solubility of hydrogen halides. See *Solubility Series* **42** (1990) which states a high precision high vacuum apparatus was used to accurately measure the change in pressure of the gas on absorption in the solvent

Source and Purity of Materials:

(1) Boron trifluoride. Purified by preparation of the anisole addition compound followed by regeneration at higher temperatures. The BF_3 vapor pressure=298 mmHg at −111.8 °C.
(2) Nitrobenzene. DuPont Technical Grade. Distilled at atm pressure and dried over CaH_2. Impurity 0.16 mol % by cooling curve analysis.

Estimated Error:

$\delta k/k=0.015$ (Compiler's estimate).

Components:

(1) Trifluoroborane; BF_3; [7637-07-2]
(2) 1,1′-Oxybis-2-chloro-ethane (chlorex); $C_4H_8Cl_2O$; [111-44-4]; or Sulfuric acid; H_2SO_4; [7664-93-9]

Variables:

T/K=278–280
p_{tot} /MPa=0.1013

Original Measurements:

A. K. Makarov and G. M. Panchenkov, Zh. Fiz. Khim. **34**, 639–40 (1960); Russ. J. Phys. Chem. (Engl. Transl.) **34**, 303–05 (1960).

Prepared By:

H. L. Clever

Experimental Values

Solubility of BF_3 in 1,1′-Oxybis-2-chloroethane (chlorex) at 5–7 °C and 1 atm total pressure

Solvent g_2 /g	BF_3 Absorbed V/cm^3 (STP)	BF_3 Solubility α/cm^3 (STP) cm^{-3}	Mol BF_3 /mol Solvent $r_{1,2}$
12.05	1980	198	0.93
11.95	1945	195	0.92
24.38	4180	209	0.97
		201 av.	

Solubility of BF_3 in sulfuric acid at 5–7 °C and 1 atm total pressure

Solvent g_2 /g	BF_3 Absorbed V/cm^3 (STP)	BF_3 Solubility α/cm^3 (STP) cm^{-3}	Mol BF_3 /mol Solvent $r_{1,2}$
45.83	3010	129	0.294
91.88	5580	110	0.267
		120 av.	

About 16 additional points are shown on a graph up to temperatures greater than 150 °C for the chlorex system 100 °C for the sulfuric acid system. The solubility decreases with increasing temperature along an 'S' shaped curve to a value near 15 cm^3 cm^{-3} at 150 °C for the chlorex and to about 50 cm^3 cm^{-3} for the acid. According to the authors the results indicate the formation of a 1:1 BF_3·chlorex complex and a $BF_3 \cdot (3\text{-}4)H_2SO_4$ complex both of which decomposes with increasing temperature.

Auxiliary Information

Method/Apparatus/Procedure:

The all glass apparatus consisted of a section I to prepare the BF_3 from boron oxide, ammonium tetraborate, and sulfuric acid, Section II to collect, store, and measure the BF_3, and Section III where gas and solvent are brought together and equilibrated. The gas not absorbed was collected in Section IV similar to the gas measuring Section II. Tetrachloromethane was used as the confining liquid in the gas measuring sections II and IV. The temperature was increased in steps of 15–20 °C and readings taken until the boiling point of the solvent was reached. The absorption of BF_3 in the CCl_4 was the source of greatest error in the procedure.

Source and Purity of Materials:

(1) Boron trifluoride. Prepared in the apparatus by dropwise addition of H_2SO_4 to a mixture of B_2O_3 and NH_4BF_4.
(2) Chlorex. Pure Grade. Dried over sodium and fractionated. Sulfuric acid. Analytical Reagent Grade. Used as received.

Estimated Error:

δT/K=±1 (compiler).
$\delta\alpha/\alpha=0.05$ (authors).

Components:
(1) Trifluoroborane; BF_3; [7637-07-2]
(2) Uranium fluoride; UF_4; [10049-14-6]
(3) Thorium fluoride; ThF_4; [13709-59-6]
(4) Beryllium fluoride; BeF_2; [7789-49-7]
(5) Lithium fluoride; LiF; [7789-24-4]

Original Measurements:
S. Cantor, J. Nucl. Mater. **47**, 177–186 (1973)

Variables:
T/K = 793.7–1044.6
p_1 /MPa = 0.0258–0.3186

Prepared By:
H. L. Clever

Experimental Values

Solubility of BF_3 in molten $LiF+BeF_2+ThF_4+UF_4$.

[Melt composition: LiF, 71.7; BeF_2, 16.03; ThF_4, 12.04; UF_4, 0.23 mol %] 0.026731 mol BF_3 charged into the vessel

Temperature		Pressure		Boron trifluoride solubility	
(t/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	Mol Fraction 10^3x_1	Henry's Constant ($10^3 K_H$ /atm^{-1})
520.5	793.7	0.255	0.0258	1.186	4.65_0
545.8	819.0	0.354	0.0359	1.175	3.31_8
571.6	844.8	0.456	0.0462	1.152	2.52_7
592.0	865.2	0.558	0.0565	1.141	2.04_5
641.2	914.4	0.851	0.0862	1.099	1.29_1
660.0	933.2	0.987	0.1000	1.079	1.09_3
714.2	987.4	1.40_5	0.1424	1.022	0.727_6
765.4	1038.6	1.93	0.1960	0.9503	0.492_4
771.4	1044.6	2.00	0.2031	0.9431	0.470_6
722.3	995.5	1.49_7	0.1517	1.010	0.674_5
674.0	947.2	1.10_8	0.1121	1.062	0.959_8
584.8	858.0	0.534	0.1121	1.144	2.14_3
549.6	822.8	0.374	0.0379	1.170	3.12_8

Solubility with 0.54 mol BF_3 charged into the vessel

Temperature		Pressure		Boron trifluoride solubility	
(t/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	Mol Fraction 10^3x_1	Henry's Constant ($10^3 K_H$ /atm^{-1})
720.8	994.0	3.05	0.309	2.036	0.667_6
688.3	961.5	2.46	0.249	2.110	0.857_7
638.5	911.7	1.76	0.178	2.216	1.25_9
522.2	795.4	0.572	0.0580	2.397	4.19_1
577.0	850.4	1.030	0.104	2.309	2.24_4
622.7	895.9	1.57	0.159	2.245	1.43_0
725.4	998.6	3.14_4	0.3186	2.040	0.648_8
602.8	876.0	1.31	0.133	2.283	1.74_3
575.2	848.4	1.31	0.103	2.315	2.27_6
533.0	806.2	0.650	0.0659	2.382	3.66_5

Solubility with 0.07907 mol BF_3 charged into the vessel

Temperature		Pressure		Boron trifluoride solubility	
(t/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	Mol Fraction (10^3x_1)	Henry's Constant (10^3K_H /atm^{-1})
623.2	896.4	2.27	0.230	3.232	1.42_4
643.7	916.9	2.69_5	0.2731	3.196	1.18_6
614.3	887.5	2.12	0.215	3.282	1.54_8
662.3	835.5	3.00	0.304	3.153	1.05_1

The 27 data points between 520 °C and 771 °C above were fitted to the equation:

$$K_H/\text{atm}^{-1} = x_1/(p_1/\text{atm}) = \exp(-14.692)\exp[7333/(T/\text{K})].$$

The author calculated from the equation the Henry constant at 1000 K of 0.000634 atm^{-1}; the enthalpy of solution, $\Delta H° = -14.5$ kcal mol^{-1} (60.9 kJ mol^{-1}); and the entropy change of transfer of BF_3 from the gas phase to the solution phase at equal concentrations, $\Delta S_C = -12.6$ cal K^{-1} mol^{-1} (-52.7 J K^{-1} mol^{-1}). Three other melts were studied. The detailed data were not given, but the data were summarized and they are given below.

Summary of BF_3 solubility in molten fluoride solvents;

Henry's constants and thermodynamic information at 1000 K

Solvent Composition, $100x_2$	Temperature Range (t/°C)	Henry's Constant Equations
1. $LiF+BeF_2$ (66-34)	498–839	$\exp(-14.949)\exp[7782/(T/\text{K})]$
2. $LiF+BeF_2+ThF_4$ (76-12-12)	647–907	$\exp(-15.083)\exp[7870/(T/\text{K})]$
3. $NaF+LiF+BeF_2+ThF_4$ ($8.02\text{-}66.2_2\text{-}14.7_2\text{-}11.0_4$)	616–755	$\exp(-15.567)\exp[9203/(T/\text{K})]$

System (See above)	Henry's Constant/1000 K	Enthalpy of Solution ($\Delta H°$/kcal mol^{-1})	Entropy of gas to liquid transfer at equal conc. (ΔS_C /cal(K mol)$^{-1}$)
1	0.772	-15.4_6	-12.9
2	0.737	-15.6_4	-13.3
3	1.72	-18.3	-14.4

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined by admitting a known amount of BF_3 into an evacuated 270 cm^3 nickel vessel containing the salts and measuring the equilibrium BF_3 pressure. The fraction of BF_3 that did not dissolve was calculated from the pressure and the vapor volume of the vessel. The vessel, containing rolling nickel balls to aid agitation, was mounted in a thermostated assembly that could be rocked. Equilibrium was assumed when no pressure change was observed with an hour of rocking.
The salt mixtures were prepared from two salt mixtures supplied by J. H. Shaffer, ORNL. The mixtures were purified by sparging with HF-H_2 at 600 °C, then by sparging with H_2 alone. Final mixtures were prepared by adding the required purified salt to the original mixtures (66-34 mol % $LiF+BeF_2$ and 76-12-12 mol % $LiF+BeF_2+ThF_4$). Impurities were: Cr, 40–54 ppm; Fe, 24–39 ppm; Ni, <5 ppm; S, <3 ppm; oxide, 160–200 ppm.

Source and Purity of Materials:
(1) Boron trifluoride. Matheson Co. Stated to be minimum 99.5 wt %. Used as received. Typical impurity analysis: SO_2, 10 ppm; sulfate, 10 ppm; SiF_4, 1–10 ppm; air, <2500 ppm. Actual mass spec. analysis at ORNL gave SiF_4, 1–10 ppm and SO_2, <1 ppm (the limit of detection).
(2) Fluoride salts. See comments in the method section.

Estimated Error:
δT/K = ±0.3; $\delta p_1/p_1$ = ±0.05 below 0.6 atm and = ±0.03 at 0.6–3.0 atm; $\delta x_1/x_1$ = ±0.02 (estimates of author).

References:
Compilers NOTE: For BF_3 solubility data in the system $LiF+BeF_2+ZrF_4+ThF_4+UF_6$ (65-28-5-1-1 mol %) see *Solubility Data Series* **45/46**, 448 (1991).

3.3. The Nitrogen Fluorides

Components:
Nitrogen fluorides
(1) Nitrogen trifluoride; NF_3; [7783-54-2] and Dinitrogen tetrafluoride; N_2F_4; [10036-18-5]
(2) Water; H_2O; [7732-18-5]

Evaluators:
Rubin Battino, Wright State University, Dayton, OH 45045 H. Lawrence Clever, Emory University, Atlanta, GA 30322.
May 2002

Evaluation

1. An evaluation of the solubility of nitrogen trifluoride in water at a partial pressure of 0.101325 MPa over the temperature interval of 278.15–323.15 K.

Ashton *et al.*[1] report ten solubility measurements from 278.15 K to 323.15 K. Dean, Finch, and Gardner[2] report five solubility values (averages from 19 measurements) between 298.21 K and 318.28 K. Three of their measurements cluster near 298 K. The Keunen coefficients of the two studies agree well. The values near 298 K agree to within 1%–1.5%, near 308 K agree to within 0.2% and near 318 K agree to within 0.8%. The 15 values were fit to the three constant Clark, Glew, and Weiss (CGW) equation and to the three constant Benson and Krause (BK) equation. Both fits were very good and are given here. The CGW equation was chosen to calculate smoothed values of the mole fraction, Ostwald coefficient and thermodynamic changes given in Table 5.

The CGW equation is:

$$\ln x_1 = -(100.7964 \pm 3.2384) + (137.7159 \pm 4.6296)/(T/100\ \mathrm{K}) + (39.7728 \pm 1.5420)\ln(T/100\ \mathrm{K}).$$

For the equation fit, $r^2 = 0.9996$ and $\sigma = 0.0058$. Since two laboratories agree well on this system and all 15 values were retained in the fit, the data are classed as recommended. The equation gives a minimum in the solubility at 346 K.

The BK equation:

$$\ln x_1 = (2.5478 \pm 0.7472) - (10070.6276 \pm 448.4188)(T/\mathrm{K})^{-1} + (1784224.3087 \pm 67191.3198)(T/\mathrm{K})^{-2}.$$

For the equation fit $r^2 = 0.9996$ and $\sigma = 00056$.

2. An evaluation of the solubility of dinitrogen tetrafluoride in water at a partial pressure of 0.101325 MPa over the temperature interval 288.15–318.15 K.

Dean, Finch, and Gardner[2] report 15 values of the Keunen coefficient of N_2F_4 in water at seven temperatures from 288.15 K to 318.28 K. This is the only paper with data on the system. Thus, an evaluation cannot be carried out. However, since the author's data appear to be reliable for the $NF_3 + H_2O$ system it was decided to prepare a table for the $N_2F_4 + H_2O$ system from their data. As above the data were fit to both the three constant CGW and BK equations. Both equations are given here, but Table 6 was constructed from the CGW equation using the seven average values at the seven temperatures.

The Clark, Glew, and Weiss (CGW) equation is:

$$\ln x_1 = -(114.3226 \pm 0.3103) + (159.9211 \pm 0.4452)/(T/100\ \mathrm{K}) + (45.4115 \pm 0.1473)\ln(T/100\ \mathrm{K}).$$

For the fit of the equation $r^2 = 0.99999$ and $\sigma = 0.0002$. A minimum in solubility is predicted by the equation to occur at 352 K.

The Benson and Krause (BK) equation:

$$\ln x_1 = (4.0144 \pm 0.1743) - (11553.5949 \pm 105.3437)(T/\mathrm{K})^{-1} + (2070444.8733 \pm 15904.8551)(T/\mathrm{K})^{-2}.$$

For the fit of the equation $r^2 = 0.99999$ and $\sigma = 0.0005$.

Since there is only one report on this system it is classed as tentative.

References

[1]J. T. Ashton, R. A. Dawe, K. W. Miller, E. B. Smith, and B. J. Stickings, J. Chem. Soc. (A), 1793–1796 (1968).
[2]C. R. S. Dean, A. Finch, and P. J. Gardner, J. Chem. Soc., Dalton Trans. 2722–2725 (1973).

TABLE 5. Smoothed recommended values of the mole fraction solubility of NF_3 in water at a partial pressure of 0.101325 MPa (1 atm) at five degree intervals from 278.15 K to 323.15 K from the CGW equation. Also given are the Ostwald coefficients and the thermodynamic changes on solution

T/K	$10^6 x_1$	Ostwald Coefficient ($10^2 L/\mathrm{cm}^3\ \mathrm{cm}^{-3}$)	$\Delta_{\mathrm{sln}}H^{\mathrm{o}}$/kJ mol^{-1}	$\Delta_{\mathrm{sln}}S^{\mathrm{o}}$/J K^{-1} mol^{-1}	$\Delta_{\mathrm{sln}}C_p{}^{\mathrm{o}}$/J K^{-1} mol^{-1}
278.15	24.79	3.14	−22.52	−169.1	331
283.15	21.16	2.73	−20.87	−163.2	331
288.15	18.25	2.73	−19.21	−157.4	331
293.15	16.01	2.13	−17.56	−151.7	331
298.15	14.27	1.93	−15.91	−146.1	331
303.15	12.91	1.77	−14.25	−140.6	331
308.15	11.84	1.65	−12.60	−135.2	331
313.15	11.01	1.56	−10.95	−129.9	331
318.15	11.01	1.49	−9.295	−124.6	331
323.15	9.85	1.43	−7.645	−119.5	331

TABLE 6. Smoothed tentative values of the mole fraction solubility of N_2F_4 in water at a partial pressure of 0.101325 MPa (1 atm) at five degree intervals from 288.15 K to 318.15 K as calculated from the CGW equation. Given also are the Ostwald coefficient and the thermodynamic changes on solution

T/K	$10^6 x_1$	Ostwald Coefficient ($10^2 L/\mathrm{cm}^3\ \mathrm{cm}^{-3}$)	$\Delta_{\mathrm{sln}}H^{\mathrm{o}}$/kJ mol^{-1}	$\Delta_{\mathrm{sln}}S^{\mathrm{o}}$/J K^{-1} mol^{-1}	$\Delta_{\mathrm{sln}}C_p{}^{\mathrm{o}}$/J K^{-1} mol^{-1}
288.15	21.15	2.77	−24.17	−173.4	378
293.15	17.93	2.39	−22.28	−173.4	378
298.15	15.48	2.10	−20.39	−160.5	378
303.15	13.60	1.87	−18.50	−154.2	378
308.15	12.15	1.70	−16.62	−148.0	378
313.15	11.02	1.56	−14.73	−141.9	378
318.15	10.14	1.46	−12.84	−141.9	378

Components:
(1) Nitrogen trifluoride; NF_3; [7783-54-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. T. Ashton, R. A. Dawe, K. W. Miller, E. B. Smith and B. J. Stickings, J. Chem. Soc. (A), 1793–1796 (1968).

Variables:
T/K = 278.2–323.2
p_1 /kPa = 80–160

Prepared By:
H. L. Clever

Experimental Values

The solubility of nitrogen trifluoride in water at 101.3 kPa (1 atm)

t/°C	T/K	$10^6 x_1$	Kuenen Coefficient/10^3 S/cm^3 g^{-1} atm^{-1}
5	278.2	25.07	31.19
10	283.2	21.03	26.17
15	288.2	18.24	22.70
20	293.2	16.10	20.03
25	298.2	14.44	17.97
30	303.2	12.84	15.94
35	308.2	11.89	14.79
40	313.2	11.00	13.69
45	318.2	10.33	12.85
50	323.2	9.82	12.22

The compiler calculated the mole fraction solubilities assuming the ideal gas volume of 22,414 cm^3 mol^{-1}.
The authors used the smoothing equation for the mole fractions:

$$\log x_1 = 5785.95/(T/\mathrm{K}) + 38.2556 \log(T/\mathrm{K}) - 118.9122$$

Note that the equations for CF_4 and SF_6 are reversed in the original paper.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is designed for the measurement of gas solubilities of the order of 10^{-6} mole fraction. It allows the bulk of the gas measurements to be performed under "dry" conditions.[1] The apparatus consists of a gas buret, a 1200 cm^3 cylindrical solution vessel with magnetically driven stirrers at the top and the bottom, and a secondary buret which also acts as a manometer. The parts are connected by 1 mm capillary tubing.
The water is degassed by boiling under vacuum for 5 h. The apparatus is evacuated and then filled. The gas and water are contacted, and the system is stirred for 12 h. Measurements are made at pressures between 600 and 1200 mmHg (80–160 kPa). Henry's law is obeyed. The solubilities at 1 atm (101.3 kPa) are obtained by interpolation.

Source and Purity of Materials:
(1) Nitrogen trifluoride. Eastman Kodak Co. Redistilled in the apparatus. Mass Spectrometry showed a purity of 99.5%.
(2) Water. Double distilled.

Estimated Error:
δT/K = ±0.02 apparatus; ±0.05 buret (precision).
$\delta S/S$ = ±0.01 (random); ±0.003 (repeat).

References:
[1] J. Horiuti, Sci. Papers Inst. Phys. Chem. Res. Tokyo, **17**, 125 (1931).

Components:
(1) Nitrogen fluoride or nitrogen trifluoride; NF_3; [7783-54-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. R. S. Dean, A. Finch, and P. J. Gardner, J. Chem. Soc., Dalton Trans. 2722-25 (1973).

Variables:
T/K = 298.21–313.28
p_1 /MPa = 0.101325

Prepared By:
H. L. Clever

Experimental Values

Solubility of nitrogen trifluoride in water at 298.21–313.28 K and 0.1013 MPa

T/K	Number of Determinations	Keunen Coefficient/10^3 k/cm^3 (STP) g^{-1}	Standard Deviation
298.21	8	17.76	0.24
298.26	1	17.25	–
298.56	1	17.60	–
308.29	5	14.82	0.07
318.28	4	12.95	0.07

The authors fitted the data to the equation: $\lg x_1 = 4596.4/(T/\mathrm{K}) + 29.558 \lg(T/\mathrm{K}) - 93.404$.
where x_1 is the mole fraction solubility and lg the base 10 logarithm.

Enthalpy and entropy of solution were calculated from the equation at 10 degree intervals from 278.15 K to 318.15 K. At 298.15 K, the values were: ΔH/kcal mol^{-1} = 3.5 and ΔS/cal K^{-1} mol^{-1} = 34.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consisted of a gas buret, a calibrated glass solution vessel of ~380 cm^3 volume attached to a length of precision bore tubing of known volume per unit length, and a high and low pressure measuring system that allowed the system to be pressurized up to ~1300 mmHg. The apparatus was in a thermostated water bath. The gas was added in the dry state to the solution vessel and its amount determined by PVT measurements and an equation of state. The water was distilled from acidified $KMnO_4$ solution and degassed by three high vacuum trap to trap distillations. The gas and water were equilibrated for about 3 h with rapid stirring with a polytetrafluoroethylene encapsulated magnetic bar. The process was repeated at a series of temperatures and pressures without further transfer of gas.

Source and Purity of Materials:
(1) Nitrogen trifluoride. Air Products Co. Purified by trap to trap distillation. Vapor pressure at 147 K checked with accepted value.
(2) Water. Distilled from acidified potassium permanganate. Further purified by trap to trap distillation.

Estimated Error:
δT/K = ±0.01.

Components:

(1) Nitrogen fluoride or nitrogen trifluoride; NF_3; [7783-54-2]
(2) Superacid solvent: HSO_3F; [7789-21-1] + SbF_5; [7783-70-2] + SO_3; [7446-11-9]
(Fluorosulfuric acid + Antimony fluoride + Sulfur trioxide)

Original Measurements:

R. J. Gillespie and G. P. Pez, Inorg. Chem. **8**, 1233–35 (1969).

Variables:

T/K = 293
p_1 /kPa = 101

Prepared By:

H. L. Clever

Experimental Values

The solubility of NF_3 in the super acid solvent, $HSO_3F + SbF_5$ ($m = 0.36$ mol kg^{-1}) + SO_3($m = 1.06$ mol kg^{-1}), is less than 1 mL of gas per 100 mL of solvent.

The solubility of the gases He, Ne, Xe, O_2, N_2, CO, CO_2, and SO_2 were also determined in the super acid solvent.

Auxiliary Information

Method/Apparatus/Procedure:

Gas solubilities were measured in the superacid solvent by following gas pressure changes accompanying dissolution in a volume calibrated system at (20 ± 0.3)°C. Ideal gas behavior was assumed.

Source and Purity of Materials:

(1) Nitrogen trifluoride. K & K Chemicals, NY. Minimum purity stated to be 95%. Stored in glass over P_2O_5 several days before use.
(2) Superacid. Prepared by mixing HSO_3F and SbF_5, then adding a 20% w/w solution of SO_3 in HSO_3F. All transfers were under dry nitrogen.

Estimated Error:

δT/K = ±0.3.
Solubility: Qualitative.

Components:

(1) Nitrogen fluoride (Nitrogen trifluoride); NF_3; [7783-54-2]
(2) Hydrogen fluoride; HF; [7664-39-3]

Original Measurements:

R. T. Rewick, W. E. Tolberg, and M. E. Hill, J. Chem. Eng. Data **15**, 527–530 (1979).

Variables:

T/K = 195.95–292.95
p_1 /kPa = 65.2–1292

Prepared By:

C. L. Young

Experimental Values

Solubility of nitrogen trifluoride in anhydrous hydrogen fluoride from 195.95 K to 292.95 K and various pressures

T/K	p_{tot} /kPa	p_1 /kPa	m_1 /mol kg^{-1}	x_1
292.95	169.3	65.2	0.0281	0.000563
292.95	370.6	269.3	0.110	0.00221
292.95	568.0	470.6	0.194	0.00392
292.95	765.3	674.6	0.277	0.00562
292.95	958.6	878.6	0.359	0.00732
292.95	1152	1085	0.440	0.00900
292.95	1343	1292	0.520	0.01069
272.94	274.6	228.0	0.112	0.00226
272.94	610.6	573.3	0.278	0.00564
272.94	674.6	638.6	0.317	0.00634
272.94	1139	1131	0.564	0.01162
195.95	94.7	94.5	0.152	0.00306
	221.3	225.3	0.307	0.00790
	240.0	254.6	0.436	0.00892
	362.6	376.0	0.680	0.01409
	414.6	429.3	0.791	0.01649
	518.6	546.6	1.05	0.02220

The compiler calculated the mole fraction solubility values.

Auxiliary Information

Method/Apparatus/Procedure:

Static equilibrium cell made of Monel metal. Known amounts of nitrogen trifluoride added to known amounts of hydrogen fluoride. Quantity of gas absorbed calculated from equilibrium pressure and cell volume.

Source and Purity of Materials:

(1) Nitrogen trifluoride. Air Products Co. Sample purity 99 mole %, reminder mainly air which was removed by pumping on liquid at −196 °C.
(2) Hydrogen fluoride. Olin Corp. Anhydrous sample. Conductivity 3×10^5 Ω^{-1} cm^{-1}.

Estimated Error:

δT/K = ±0.02.
$\delta x_1 / x_1$ = ±0.03 (estimated by compiler).

Components:

(1) Nitrogen fluoride or nitrogen tetrafluoride; N_2F_4; [10036-47-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. R. S. Dean, A. Finch and P. J. Gardner, J. Chem. Soc., Dalton Trans. 2722–25 (1973).

Variables:

T/K = 288.15–318.18
p_1 /MPa = 0.101325

Prepared By:

H. L. Clever

Experimental Values

Solubility of nitrogen tetrafluoride in water at 288.15–318.18 K and 0.1013 MPa

T/K	Keunen Coefficient $10^3\ k/\mathrm{cm}^3$ (STP) g^{-1} (Experimental)	Keunen Coefficient $10^3\ k/\mathrm{cm}^3$ (STP) g^{-1} (corrected)	Keunen Coefficient $10^3\ k/\mathrm{cm}^3$ (STP) g^{-1} (calculated)
288.15	27.32	26.42	26.22
289.15	25.59	24.77	—
289.15	26.26	25.53	25.33
298.11	19.96	19.07	—
298.11	20.14	19.21	—
298.11	20.19	19.21	19.21
298.16	19.15	19.10	—
298.16	19.42	19.32	—
298.16	19.67	19.55	19.18
298.26	19.15	19.08	19.13
308.09	15.46	14.88	—
308.09	15.79	15.11	15.07
318.28	12.88	12.55	—
318.28	12.95	12.55	—
318.28	13.14	12.61	12.56

The authors fitted the corrected (see below) data to the equation:

$$\lg x_1 = 6936.9/(T/\mathrm{K}) + 45.435 \lg(T/\mathrm{K}) - 140.28$$

where x_1 is the mole fraction solubility and lg the base 10 logarithm.

Enthalpy and entropy of solution were calculated from the equation at 10 degree intervals from 278.15 K to 318.15 K. At 298.15 K the values are: ΔH/kcal mol^{-1} = 4.9 and ΔS/cal K^{-1} mol^{-1} = 38.

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus consisted of a gas buret, a calibrated glass solution vessel of ~380 cm^3 volume attached to a length of precision bore tubing of known volume per unit length, and a high and low pressure measuring system that allowed the system to be pressurized up to ~1300 mmHg. The apparatus was in a thermostated water bath. The gas was added in the dry state to the solution vessel and its amount determined by PVT measurements and an equation of state. The water was distilled from acidified $KMnO_4$ solution and degassed by three high vacuum trap to trap distillations. The gas and water were equilibrated for about 3 h with rapid stirring with a polytetrafluoroethylene encapsulated magnetic bar. A slow reaction during the equilibration was corrected for using data from Hurst and Khayat.[1]

Source and Purity of Materials:

(1) Nitrogen tetrafluoride. Air Products Co. Research Grade. Treated with Br_2 and purified by trap to trap distillation to remove suspected NF_2NO. Purity checked by I. R. and vapor pressure.
(2) Water. Distilled from acidified potassium permanganate. Further purified by trap to trap distillation.

Estimated Error:

δT/K = ±0.01.

References:

[1]G. L. Hurst and S. I. Khayat, Adv. Chemistry Series No. **54**, 245 (1966).

TABLE 7. Smoothed tentative values of the mole fraction solubility at one 0.101325 MPa (1 atm) partial pressure, Ostwald coefficient and thermodynamic changes of solution as a function of temperature between 273.15 K and 473.15 K

Temperature (T/K)	Mole Fraction $10^6 x_1$	Ostwald Coefficient ($10^2 L/\mathrm{cm}^3\ \mathrm{cm}^{-3}$)	Enthalpy Change ($\Delta_{sol}H$/kJ mol^{-1})	Entropy Change ($\Delta_{sol}S$/J K^{-1} mol^{-1})	Heat Capacity Change ($\Delta_{sol}C_p$ /J K^{-1} mol^{-1})
273.15	11.080	1.378	−29.19	−201.7	312.7
278.15	8.848	1.121	−27.63	−196.1	312.7
283.15	7.208	0.929	−26.07	−190.5	312.7
288.15	5.982	0.784	−24.50	−185.0	312.7
293.15	5.052	0.673	−22.94	−179.6	312.7
298.15	4.338	0.587	−21.38	−174.4	312.7
303.15	3.782	0.520	−19.81	−169.2	312.7
308.15	3.346	0.467	−18.25	−164.0	312.7
313.15	3.001	0.425	−16.69	−159.0	312.7
318.15	2.726	0.391	−15.12	−154.1	312.7
323.15	2.507	0.365	−13.56	−149.2	312.7
333.15	2.192	3.470	−10.44	−139.7	312.7
343.15	1.996	0.305	−7.309	−130.4	312.7
353.15	1.885	0.295	−4.187	−121.4	312.7
363.15	1.839	0.294	−4.187	−112.7	312.7
373.15	1.839	0.301	+2.069	−104.2	312.7
383.15	1.904	0.317	5.195	−95.9	312.7
393.15	2.010		8.321	−87.7	312.7
403.15	2.166		11.45	−80.0	312.7
413.15	2.379		14.57	−72.4	312.7
423.15	2.658		17.70	−64.9	312.7
433.15	3.016		20.63	−57.6	312.7
443.15	3.470		23.95	−50.5	312.7
453.15	4.043	—	27.08	−43.5	312.7
463.15	4.764	—	30.16	−36.7	312.7
473.15	5.671	—	33.27	−30.0	312.7

3.4. (O–C-6-11)-Sulfur Fluoride

Components:

(1) Sulfur fluoride or Sulfur hexafluoride; SF_6; [2551-62-4]
(2) Water; H_2O; [7732-16-5]

Evaluators:

Rubin Battino, Wright State University, Dayton, OH 45435.
H. Lawrence Clever, Emory University, Atlanta, GA 30322. June 2003

Evaluation

An evaluation of the solubility of sulfur fluoride, SF_6, in water at a partial pressure of 0.101325 MPa from 273.15 K to 473.15 K

The solubility of sulfur hexafluoride is reported in 18 papers. The data of two papers were not used. The remaining sixteen papers contain 79 experimental values of the solubility of SF_6 in water. The data were fitted by a nonlinear regression to both the three and four constant Clark, Glew, and Weiss (CGW) equation and the Benson and Krause (BK) equation. The CGW equation is a van't Hoff type equation and the BK equation is an inverse temperature power series. The procedure is to carry out the nonlinear regression on all of the data, discard any points that fall 2 s.d. or more from the regression line and refit the remaining points. This is repeated until all remaining points are within 2 s.d. of the regression line. The total experimental values and the number of experimental values in the final regression are summarized below.

Reference Number	Total Number of Experimental Values	Number of Experimental Values Used in the Final Nonlinear Regression
1	3	2
2	7	2
3	15	11
4	4	0
5, 6	1	1
7	—	Not used (graphical data)
8, 10	1	0
9	1	0
11	8	3
12	2	Not used (graphical data)
13	1	1
14, 15	3	0
16	9	4
17	31	17
18	1	1

The three constant CGW equation was chosen to represent the data. The equation is:

$$\ln x_1 = -(99.6463 \pm 1.9018) + (137.8146 \pm 2.9271)/(T/100\ \text{K}) + (37.5997 \pm 0.8389)\ln(T/100\ \text{K})$$

with x_1 the mole fraction solubility at 0.101325 MPa (1 atm) partial pressure and (T/100 K) the Kelvin temperature divided by 100. From the equation fit, $r^2 = 0.9881$ and the standard error of estimate is 0.0454 in $\ln x_1$.

Table 7 gives smoothed values of the mole fraction solubility at five degree intervals from 273.15 K to 323.15 K and at ten degree intervals from 323.15 K to 473.15 K. Also given are values of the Ostwald coefficient and the thermodynamic changes for solution of enthalpy, entropy, and heat capacity. The equation predicts a minimum in the solubility at 367 K.

Figure 1 follows the references. It shows the fitted line and many of the experimental values on an $\ln x_1$ vs T/100 K plot.

References

[1]H. L. Friedman, J. Am. Chem. Soc. **76**, 3294–3297 (1954).
[2]T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).
[3]J. T. Ashton, R. A. Dawe, K. W. Miller, E. B. Smith, and B. J. Stickings, J. Chem. Soc. (A) 1793–1796 (1970).
[4]S. K. Shoor, R. D. Walker, Jr., and K. E. Gubbins, J. Phys. Chem. **73**, 312–317 (1969).
[5]G. G. Power and H. Stegall, J. Appl. Physiology **29**, 145–146 (1970).
[6]L. D. Longo, M. Delivoria-Papadopoulos, G. G. Power, E. P. Hill, and R. E. Forster, Am. J. Physiology **219**, 561–569 (1970).
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[8]M. Meyer, Pflügers Arch. **375**, 161 (1978).
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[11]B. A. Cosgrove and J. Walkley, J. Chromatogr. **216**, 161–167 (1981).
[12]R. A. Smith, E. G. Porter and K. W. Miller, Biochem. Biophys. Acta **645**, 327–338 (1981).
[13]T. Park, T. R. Rettich, R. Battino, D. Peterson and E. Wilhelm, J. Chem. Eng. Data **27**, 324–326 (1982)
[14]R. Guitart, A. Puigdemont and M. Arboix, J. Chromatog. **491**, 271–280 (1989).
[15]R. Guitart, Reviste Espanola de Fisiologia **49**, 195 202 (1993).
[16]E. K. Mroczek, J. Chem. Eng. Data **42**, 116–119 (1997).
[17]J. L. Bullister, D. P. Wisegarver and F. A. Menzia, Deep-Sea Research, Part I: Oceanographic Research Papers **49**(1), 175–187 (2002).
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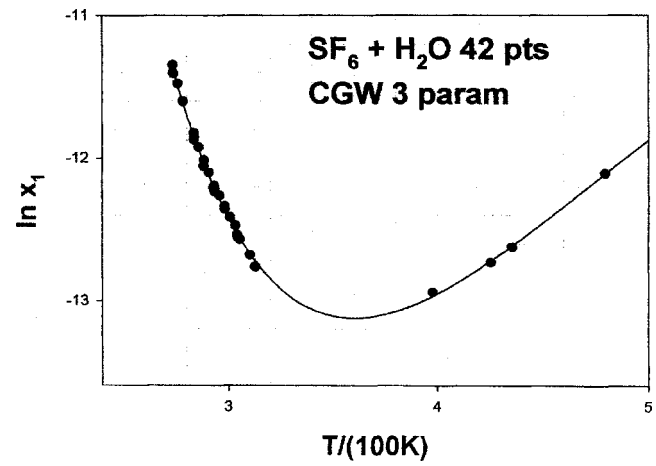


FIG. 1. The solubility of SF_6 in H_2O: $\ln x_1$ vs $T/(100\ \text{K})$. The fitted curve and experimental points used.

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Nitromethane; CH_3NO_2 ; [75-52-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
H. L. Friedman, J. Am. Chem. Soc. **76**, 3294–97 (1954).

Variables:
T/K = 273.25, 288.05, and 298.00
p_1 /kPa = 93.33 (700 mmHg)

Prepared By:
H. L. Clever

Experimental Values

Solubility of sulfur hexafluoride in water

Temperature (t/°C)	(T/K)	Mol Fraction $10^5 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
0.1	273.25			0.0147
0.1	273.25			0.0147
0.1	273.25	1.18	0.0147	0.0147 av.
14. 9	288.05			0.0076
14. 9	288.05			0.0076
14. 9	288.05	0.58	0.0072	0.0076 av.
24.85	298.00			0.0054
24.85	298.00			0.0053
24.85	298.00			0.0055
24.85	298.00			0.0058
24.85	298.00	0.41	0.0050	0.0055 av.

Solubility of sulfur hexafluoride in nitromethane saturated water

Temperature (t/°C)	(T/K)	Mol Fraction $10^5 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
24.85	298.00			0.0058
				0.0053
			0.0050	0.0055 av.

The compiler calculated and added the Kelvin temperatures, the Bunsen coefficients, and mole fraction values. The solubility calculations were made for a partial pressure of 101.325 kPa (760 mmHg) assuming Henry's law and ideal gas behavior. The nitromethane saturated water contained about 4 mol % nitromethane.[3]

Auxiliary Information

Method/Apparatus/Procedure:
The gas absorption method was essentially that employed by Euken and Herzberg.[1] Their method was modified by the use of a magnetic stirrer, and by use of electrical contacts in the mercury manometer to aid balancing the pressure.
The solvent was degassed by vacuum. The procedure, repeated 5–10 times, was to alternate 5–15 s evacuation and rapid stirring to produce cavitation. In the solubility measurement, gas presaturated with solvent vapor, was brought into contact with about 80 cm^3 of solvent in the saturation vessel. Initial conditions were established by a time extrapolation. Solubility was approached from both under- and super-saturation.
See also the data sheet (compilation page) of sulfur hexafluoride + nitromethane from this paper.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Fractionally condensed at 83.15 K. Vapor pressure 275–6 mmHg at 195.15 K agrees with literature valu.[2]
(2) Water. Conductivity water.

Estimated Error:
δT/K = ±0.05.
δp_1 /mmHg = ±0.3.
$\delta L/L$ = ±0.03.

References:
[1]A. Euken and G. Herzberg, Z. Phys. Chem. **1**, 195 (1950).
[2]W. C. Schumb, Ind. Eng. Chem. **39**, 421 (1947).
[3]R. M. Corelli, Aerotecnica **30**, 32 (1950); Chem. Abstr. **46**, 3370e (1952).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).

Variables:
T/K = 284.1–302.8
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of sulfur hexafluoride in water between 10.9 °C and 29.6 °C at a partial pressure of 1 atm

t/°C	T/K	Solubility S [S/cm^3 (STP) g^{-1} atm^{-1}]	Mole fraction solubility $10^6 x_1$
10.9	284.1	7.9	6.3
12.5	285.7	7.4	5.9
14.2	287.4	7.0	5.6
19.6	292.8	6.2	5.0
25.0	298.2	5.4	4.3
25.0	301.0	5.2	4.2
29.	302.8	5.1	4.1

The solubility, S, is 1000 times the Kuenen coefficient. The compiler calculated mole fraction solubilities assuming ideal gas behavior and Henry's law. The compiler also added the Kelvin temperatures.

Auxiliary Information

Method/Apparatus/Procedure:
The degassed water flows in a thin film down a glass helix absorption tube containing the sulfur hexafluoride gas and water vapor at a total pressure on one atm (101.3 kPa). The volume of gas absorbed is measured in an attached buret system.[1]

Source and Purity of Materials:
(1) Sulfur hexafluoride. Imperial Chemical Industries Ltd. Purity not specified.
(2) Water. Nothing specified.

Estimated Error:
$\delta S/S$ = ±0.03

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948); J. Chem. Soc. 3819 (1952).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. T. Ashton, R. A. Dawe, K. W. Miller, E. B. Smith, and B. J. Stickings, J. Chem. Soc. (A), 1793–1796 (1968).

Variables:
T/K = 275.7–323.2
p_1 /kPa = 80–160

Prepared By:
H. L. Clever

Experimental Values

Solubility of sulfur hexafluoride in water at 101.3 kPa (1 atm)

t/°C	T/K	$10^6 x_1$	Kuenen Coefficient (10^3 S/cm^3 g^{-1} atm^{-1})
2.5	275.7	10.34	12.86
5.0	278.2	9.12	11.35
10.0	283.2	7.34	9.13
12.5	285.7	6.61	8.23
15.0	288.2	6.04	7.51
17.5	290.7	5.55	6.90
20.0	293.2	5.05	6.28
22.5	295.7	4.73	5.88
25.0	298.2	4.38	5.45
27.5	300.7	4.07	5.07
30.0	303.2	3.83	4.76
35.0	308.2	3.45	4.29
40.0	313.2	3.21	3.99
45.0	318.2	3.00	3.73
50.0	323.2	2.83	3.52

The compiler calculated the mole fraction solubility assuming the ideal gas volume of 22 414 cm^3 mol^{-1}.
The authors used the smoothing equation for the mole fractions:

$$\log x_1 = 9116.79/(T/\mathrm{K}) + 62.2675 \log(T/\mathrm{K}) - 199.0132$$

Note that the equations for CF_4 and SF_6 are reversed in the original paper.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is designed for the measurement of gas solubilities of the order of 10^{-6} mole fraction. It allows the bulk of the gas measurements to be performed under "dry" conditions.[1] The apparatus consists of a gas buret, a 1200 cm^3 cylindrical solution vessel with magnetically driven stirrers at the top and the bottom, and a secondary buret which also acts as a manometer. The parts are connected by 1 mm capillary tubing.
The water is degassed by boiling under vacuum for 5 h. The apparatus is evacuated and then filled. The gas and water are contacted, and the system is stirred for 12 h. Measurements are made at pressures between 600 and 1200 mmHg (80–160 kPa). Henry's law is obeyed. The solubilities at 1 atm (101.3 kPa) is obtained by interpolation.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Imperial Smelting Co. Redistilled in the apparatus. Mass Spectrometry showed a purity of 99.9%.
(2) Water. Double distilled.

Estimated Error:
δT/K = ±0.02 apparatus; ±0.05 buret (precision).
$\delta S/S$ = ±0.01 (random); ±0.003 (repeat).

References:
[1]J. Horiuti, Sci. Papers Inst. Phys. Chem. Res. Tokyo, **17**, 125 (1931).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Potassium hydroxide; KOH; [1310-58-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
S. K. Shoor, R. D. Walker, Jr. and K. E. Gubbins, J. Phys. Chem. **73**, 312–317 (1969).

Variables:
T/K = 298.15–353.15
p_1 /kPa = 101.325
c_2 /mol L^{-1} = 0–7.35

Prepared By:
H. L. Clever

Experimental Values

T/K	KOH 100 w_2	KOH* (c_2 /mol L^{-1})	Gas Mol Fraction** $10^5 x_1$	Solubility ratio $\gamma = x^o_1/x_1$	Salt Effect Parameter (k_{scx} /L mol^{-1})
298.15	0.0	0.0	0.40	1.00	—
298.15	5.00	0.92		2.15	0.361
298.15	13.50	2.67		7.44	0.405
298.15	23.00	5.00		43.2	0.327
298.15	31.6	7.35		234	0.322
298.15					0.326 (authors)
313.15	0.0	0.0	2.74	1.00	—
313.15	5.00	0.92		1.97	0.320
313.15	13.50	2.67		6.53	0.305
313.15	23.00	5.00		31.9	0.301
313.15	31.6	7.35		146	0.294
313.15					0.297 (authors)
333.15	0.0	0.0	2.20	1.00	—
333.15	5.00	0.92		1.88	0.298
333.15	13.50	2.67		5.88	0.288
333.15	23.00	5.00		26.6	0.285
333.15	31.6	7.35		112	0.279
333.15					0.278 (authors)
353.15	0.0	0.0	1.91	1.00	—
	5.00	0.92		1.73	0.259
	13.50	2.67		4.91	0.259
	23.00	5.00		22.6	0.271
	31.6	7.35		84.2	0.262
					0.262 (authors)

*The c_2 values measured at 298.15 K.
Compiler's NOTE: There appears to be **a decimal error in the mole fraction solubilities in the KOH solutions. They appear to be too large by a factor of 10. The values above should be 0.274, 0.220 and 0.191 × 10^{-5}.

Auxiliary Information

Method/Apparatus/Procedure:
A gas chromatographic method[1] was used. The gas saturated solution were prepared by bubbling the gas through presaturators and then the KOH solution. Samples were drawn over a 48 h period to determine when saturation was reached. Samples were transferred from the saturator to the GLC in gas tight syringes. All analyses were made with a thermal conductivity cell with N_2 as the carrier gas.
The results are reported as activity coefficients which are the mole fraction solubility ratio x_1^o/x_1 with x_1^o the mole fraction in water and x_1 the mole fraction solubility in the KOH solution. Both mole fractions were corrected to 1 atm partial pressure assuming Henry's law is obeyed. The γ's are the average of at least four measurements. The compiler calculated the k_{scx} values at the individual KOH concentrations. The overall value of the authors is also given.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Source not given, minimum purity stated to be 98.0%.
(2) Potassium hydroxide. Baker Analyzed Reagent Grade. Contained a maximum of 1% K_2CO_3. The solutions were protected from atm CO_2 by Ascarite.
(3) Water. Specially distilled and degassed from a glass-Teflon still.

Estimated Error:
δT/K = ±0.05.
$\delta\gamma/\gamma$ = ±0.01.

Note: k_{scx} /L mol^{-1} = [1/(c_2 /mol L^{-1})] log(x_1^o/x_1)

References:
[1]K. E. Gubbins, S. N. Carden, and R. D. Walker, Jr., J. Gas Chromatog. **3**, 98 (1965).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
G. G. Power and H. Stegall, J. Appl. Physiology **29**, 145–149 (1970).

Variables:
T/K = 310.15

Prepared By:
C. L. Young

Experimental Data

T/K	Bunsen Coefficient [α/cm^3 (STP) cm^{-3}]	Standard Deviation	Number of Measurements
310.15	0.00386	0.00001	3

Auxiliary Information

Method/Apparatus/Procedure:
Five to 12 cm^3 samples placed in a stirrer cell and gas, saturated with water vapor, passed through the water for 30–60 m. Samples of saturated liquid withdrawn and transferred to Van Slyke apparatus. Dissolved gas removed under reduced pressure.

Source and Purity of Materials:
(1) Sulfur Hexafluoride. Matheson Co. Purity 98 mole % minimum.
(2) Water. Nothing specified.

Estimated Error:
δT/K = ±0.1.

Components:
(1) Sulfur fluoride or sulfur hexafluoride SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. D. Longo, M. Delivia-Papadopoulos, G. G. Power, E. P. Hill, and R. E. Forster, Am. J. Physiology **219**, 561–569 (1970).

Variables:
T/K = 310.15

Prepared By:
C. L. Young

Experimental Data

T/K	Bunsen Coefficient [α/cm^3 (STP) cm^{-3}]	Standard Deviation
310.15	0.00386	0.00001

The compiler suspects this and the solubility value above are two reports of the same experiment.

Auxiliary Information

Method/Apparatus/Procedure:
Liquid samples were equilibrated with gas and then the dissolved gas was stripped out under vacuum and measured in a manometric Van Slyke apparatus. Some details in Power.[1]

Source and Purity of Materials:
Nothing specified.

Estimated Error:
δT/K = ±0.03.

References:
[1]G. G. Power, J. Appl. Physiology **24**, 468 (1968).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]
(2) Seven normal alcohols

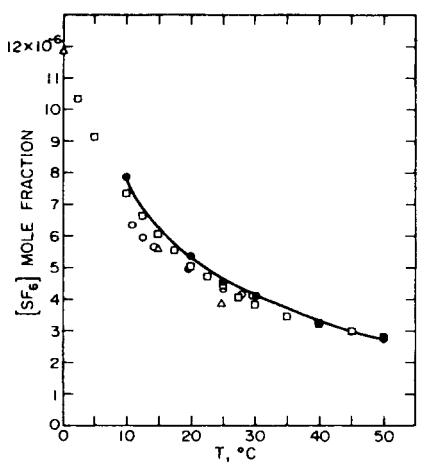
Original Measurements:
B. K. Lamb and F. H. Shair, Anal. Chem. **48**, 473–475 (1976).

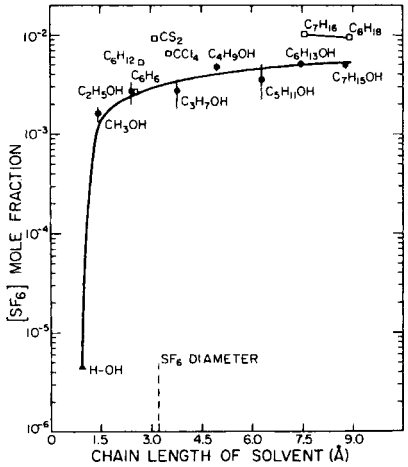
Variables:
T/K = 283–323 (H_2); 298 (alcohols)
p_1 /kPa = (barometric − solvent vapor pressure)

Prepared By:
H. L. Clever

Experimental Values

There are no numerical data. All results are in two figures reproduced below. The left figure shows the solubility of SF_6 in water from 283 K to 323 K at 1 atm total pressure. The right figure shows the logarithm of SF_6 mole fraction, $\lg x_1$, at 298 K and 1 atm total pressure in seven normal alcohols (C_1–C_7) vs solvent chain length.





Left figure. Solid circles and line, present work. Open circles, Ashton *et al.*[1] open squares, Morrison and Johnstone;[2] open triangles, Friedman.[3] Right figure. Solid circles and line, present work. Open squares, Battino and Wilhelm.[4] (Figures by permission of the American Chemical Society.)

Auxiliary Information

Method/Apparatus/Procedure:
Electron capture gas chromatography. Degassing was not necessary. Four mL of SF_6 gas and 1 mL of H_2O were drawn into a 5 mL syringe and shaken on a carousel. The gas pressure was (atm p − water vap p). Tests showed 20 m rotation saturated the solutions, 40 m were used to insure saturation. The samples were diluted with 3 times their volume of water prior to injection into the chromatograph. A 1 μL sample was added to a 6 in. Lucite cube, the water evaporates and N_2 gas flowing 120 mL m^{-1} mixes with the SF_6 and is sampled. The dilution is exponential, the initial concentration is found.
There is more detail in original paper.

Source and Purity of Material:
(1) Sulfur hexafluoride. Matheson Co. Purity not stated.
(2) Water. Distilled from lab supply.
(2) Alcohols. Either Aldrich Chemical Co. or Matheson, Coleman and Bell. Spectro-quality.

Estimated Error:
$\delta x_1 / x_1 = 0.12$ max, 0.06 Av. Std. Dev. for water;
$= 0.20$ max, 0.20 Av. Std. Dev. for alcohols.

References:
[1]T. J. Ashton, R. A. Dawes, K. W. Miller, E. B. Smith, and B. J. Stickings, J. Chem. Soc. A 1793 (1968).
[2]T. J. Morrison and N. N. B. Johnstone, J. Chem. Soc. 3655 (1955).
[3]H. L. Friedman, J. Am. Chem. Soc. **76**, 4394 (1954).
[4]R. Battino and E. Wilhelm, Chem. Rev. **73**, 1 (1973).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. P. Hlastala, M. Meyer, G. Riepl, and P. Scheid, Undersea Biomed. Res. **7**, 297–304 (1980).

Variables:
T/K = 310

Prepared By:
C. L. Young

Experimental Data

Solubility of sulfur hexafluoride in water at 37 °C

t/°C	T/K	Bunsen Coefficient [α/cm^3 (STP) cm^{-3}]	No. of Determinations	Standard Error on Mean
37	310	0.00348	30	0.00003

Auxiliary Information

Method/Apparatus/Procedure:
Aliquots were equilibrated for 60 m in a rotating tonometer with a humidified gas mixture (70% SF_6 and 30% Ar). Samples were withdrawn in a gas tight syringe and injected into a glass vessel. Partial pressure and gas phase composition estimated using mass spectrometer. Bunsen coefficients were calculated assuming Henry's law and ideal gas law obeyed.

Source and Purity of Materials:
Nothing specified.

Estimated Error:
δT/K = ±0.1 (estimated by compiler).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. Guitart, A. Puigdemont, and M. Arboix J. Chromatog. **491**, 271–280 (1989).

Variables:
T/K = 310

Prepared By:
H. L. Clever

Experimental Data

Solubility of sulfur hexafluoride in water at 37 °C

t/°C	T/K	Partition Coefficient Water/Gas [c_1 liq]/[c_1 gas]	Number of Determinations	Coefficient of Variation (%)
37	310	0.0037 ± 0.0001	8	2.7

The analysis was carried out on a mixture of gases (ethane, cyclopropane, sulfur hexafluoride, acetone, diethyl ether, and enflurane).
The Partition Coefficient is numerically equal to the Ostwald Coefficient.

Auxiliary Information

Method/Apparatus/Procedure:
A modification of the headspace gas chromatography method of Wagner *et al.*[1] was used. It used a smaller volume and fewer equilibration steps.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Abello-Oxigeno Linde. Pure grade.
(2) Water. Nothing specified.

Estimated Error:
Nothing specified.

References:
[1]P. D. Wagner, P. F. Naumann, and R. B. Laravuso, J. Appl. Physiol. **36**, 600 (1974).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Dog blood and Skeletal muscle.

Original Measurements:
M. Meyer, U. Tebbe, and J. Piiper, Pflügers Arch. **384**, 131–134 (1980).

Variables:
T/K = 310
p_1 /kPa = 101.3

Prepared By:
C. L. Young

Experimental Values

Solubility of sulfur hexafluoride in dog blood at 310 K and total pressure 101.3 kPa

Solvent	Number of Determinations	Number of Dogs	Solubility (S/μmol dm^{-3} kPa^{-1})	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]
Water	12	—	1.60 ± 0.01	0.0036
Saline	12	—	1.54 ± 0.002	0.0035
Blood	50	10	2.62 ± 0.05	0.0059
Plasma	30	10	1.73 ± 0.03	0.0039
Red cells	—	10	3.70 ± 0.09	0.0084
Muscle	39	13	5.52 ± 0.23	0.0125

The solubility of water was also reported in an earlier paper, Meyer.[1]
The saline is aqueous normal saline containing 0.154 mol NaCl L^{-1}.
Heparinized blood samples were from mongrel dogs that had fasted for 16 h.
The plasma was obtained by centrifugation of whole blood. No sign of hemolysis was observed.
The solubility in the red cells was calculated from the values for whole blood and plasma of the same animal by volume-weighted subtraction.
Muscle was gastrocnemius muscle excised from dogs, which had been anesthetized for about 6–8 h and killed by bleeding. Blood allowed to drain from a major muscle. Muscle samples homogenized.

Composition of dog blood

Component	Mean value ± Std. Dev.
Hemocrit %	45 ± 4.5
Hemoglobin (g/100 mL blood)	16.9 ± 1.6
Plasma protein (g/100 mL plasma)	6.2 ± 0.5
Total lipids (mg/100 mL plasma)	519 ± 118
Triglycerides (mg/100 mL plasma)	108 ± 82
Cholesterol (mg/100 mL plasma)	202 ± 68

Auxiliary Information

Method/Apparatus/Procedure:
Method involved equilibration of solvent with humidified gas at stated temperature and pressure and subsequent estimation of the amount of gas dissolved in a 2.5 cm^3 sample. The gas dissolved was estimated using an equilibration technique for partial extraction of gas. Quantitative analysis of extracted gas was performed by GC using helium as the carrier gas. Details are given in an earlier paper.[1]

Source and Purity of Material:
(1) Sulfur hexafluoride. Nothing specified
(2) See information of components below table on first page.

Estimated Error:
δT/K = ±0.5 (estimate by compiler).

References:
[1]M. Meyer, Pflügers Arch. **375**, 161 (1978).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Cosgrove and J. Walkley, J. Chromatogr. **216**, 161–167 (1981).

Variables:
T/K = 278.15–313.15
P_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Mole fraction solubility of sulfur hexafluoride in water from 278.15 K to 313.15 K at 1 atm (101.325 kPa) partial pressure.

T/K	$10^4 x_1$
278.15	0.09164
283.15	0.07340
288.15	0.06035
293.15	0.05143
298.15	0.04426
303.15	0.03872
308.15	0.03486
313.15	0.03226

Auxiliary Information

Method/Apparatus/Procedure:
A 20 mL volume of degassed (sublimation technique) solvent is transferred to a previously evacuated (10^{-4} mm Hg) saturation cell immersed in an insulated, controlled (±0.01 K) water bath. The gas is dispersed through the constantly stirred solution at 1 atm by a course, fritted glass disc. Saturation is obtained within a few hours. Prior to analysis the solution is allowed to sit under 1 atm gas pressure for 1 hour.
A saturated solution is withdrawn from the cell using a greaseless, gas tight Gilmont syringe of 2.500 ± 0.001 mL volume. A 0.250 mL sample is injected to "wet" the frit. It is stripped and then four 0.500 mL samples are injected sequentially into the frit of the gas chromatograph. The stripped gas is dried before entering the column. The gas is analyzed on a dual filament conductivity detector. Calibrations with pure gas are made dry before and wet after each series of runs.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Nothing specified.
(2) Water. Nothing specified.

Estimated Error:
δT/K = ±0.01.
$\delta x_1 / x_1$ = ±0.015 (Estimate of compiler).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5] or Buffer or Two Lipid biolayers (sonicated vesicles)

Original Measurements:
R. A. Smith, E. G. Porter, and K. W. Miller, Biochim. Biophys. Acta **645**, 327–338 (1981)

Variables:
T/K = 284.7, 298.2
p_1 /MPa = 0.44–1.69

Prepared By:
H. L. Clever

Experimental Data

t/°C	T/K	Range of Partial Pressure (p_1 /atm)	Bunsen Coefficient (α/cm^3(STP)cm^{-3} atm^{-3})
Water; H_2O; [7732-18-5] (See Stoelting and Longshore[1])			
10.6	283.8	4.3–16.7	0.00889
25.0	298.2	4.3–16.7	0.00546
Buffer {0.15 mol L^{-1} KCl; [7447-40-7], 0.1 mass% Na(N_3); [26628-22-8], 10 mmol L^{-1} Tris-HCl; [1185-53-1]; pH 7.4}			
10.6	283.8	4.3–16.7	0.00793
25.0	298.2	4.3–16.7	0.00496
Egg phosphatidylcholine, 96% phosphatidic acid, 4% (PC/PA)			
10.6	283.8	4.3–16.7	0.298
25.0	298.2	4.3–16.7	0.238
Egg phosphatidylcholine, 64% phosphatidic acid, 3% cholesterol; [57-88-5], 33% (PC/PA/Chol)			
10.6	283.8	4.3–16.7	0.200
25.0	298.2	4.3–16.7	0.218

Auxiliary Information

Method/Apparatus/Procedure:
Author's apparatus II. Six 18 mL glass cuvetts, each with a Teflon coated stirring button with a stainless steel wire that broke the surface, are mounted inside a 50 mm I>D> pressure cylinder. Six stainless steel tubes, 0.26 μL mm^{-1}, passed through the disc top of the pressure vessel with one tube going to the bottom of each cuvett. The cuvetts contained either water, buffer or one of the two phospholipid suspensions. The pressure chamber was flushed with the gas, then sealed and pressurized with the gas. After 12 h equilibration the cuvetts were sampled in turn by slowly bleeding 0.75 mL of solution at 0.5 mL min^{-1} through a 300 μL sample loop with a micrometer metering valve. The sample loop was decompressed and its contents flushed into a stripping device. The stripped gas went to a gas chromatograph for analysis. More on the method in Miller *et al.*[2]

Source and Purity of Materials:
(1) Sulfur hexafluoride. Nothing specified.
(2) Water and buffer. Nothing specified. Egg phosphatidylcholine and egg phosphtidic acid. Lipid Products, Nutfield. Cholesterol. Sigma Chemical Co. Recrystallized from methanol. The phospholipids with or without cholesterol were dried down from $CHCl_3$ solution and suspended in the buffer by vortexing and then sonication, centrifugation yielded translucent suspensions of 10–46 mg mL^{-1}.

Estimated Error:
δT/K = ±0.1.
$\delta\alpha/\alpha$ = ±0.035–0.05 (complier).

References:
[1]R. K. Stoelting and R. E. Longshore, Anestheisology **36** 503 (1972).
[2]K. W. Miller, L. Hammond, and E. Porter, Chem. Phys. Lipids **20**, 229 (1977).

Components:
(1) (OC-6-11)-Sulfur fluoride or Sulfur hexafluoride; SF_6; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. Park, T. R. Rettich, R. Battino, D. Peterson, and E. Wilhelm, J. Chem. Eng. Data **27**, 324–326 (1982).

Variables:
T/K = 298.15
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

Solubility of sulfur hexafluoride in water at 298.15 K and 101.325 kPa partial pressure

T/K	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]	Number of Determinations	Standard Deviation (%)
298.15	0.005440	3	1.3

Auxiliary Information

Method/Apparatus/Procedure:
Two different versions of the Scholander[1] micogasometric apparatus were used. They were housed in an air bath.
Version 1 was the modified form described by Douglas[2] and by others.
Version 2 was modified by the authors. The design includes a more efficient method of degassing and transferring water to the apparatus. The apparatus itself has a 4 cm^3 compensation chamber, a 10 cm^3 equilibrium chamber, and an 8 cm^3 side arm.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Minimum mol % purity is 99.9.
(2) Water. House distilled (reverse osmosis), passed through an ion exchange column until specific resistance was 5×10^4 S^{-1} cm.

Estimated Error:
δT/K = ±0.05.
Solubility, see percent standard deviation above.

References:
[1]P. F. Scholander, J. Biol. Chem. **167**, 235 (1947).
[2]E. Douglas, J. Phys. Chem. **68**, 169 (1964).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6; [2551-64-2]
(2) Water; H_2O; [7732-18-5]
(2) Normal saline (0.9 mass % Sodium Chloride; NaCl; [7647-14-5])
(2) 5% aqueous Glucose; $C_6H_{12}O_6$; [50-99-7]

Original Measurements:
R. Guitart, Revista Espanola de Fisiologia **49**, 195–202 (1993).

Variables:
T/K = 303.2, 310.2, and 318.2

Prepared By:
H. L. Clever

Experimental Values

Solvent	T/K	Partition Coefficient	Number of Observations	Standard Deviation
Water	303.2	0.0041	8	0.0003
Water	310.2	0.0037	8	0.0001
Water+ Sodium Chloride (0.9 mass %)	318.2	0.0034	8	0.0003
Water+ Glucose (5 mass %)	310.2	0.0031	8	0.0002
Water+ Glucose (5 mass %)	310.2	0.0032	8	0.0003

The 310.2 K value in water is from an earlier paper, Guitart *et al.*[1]

Water+ Sodium Chloride (0.9 mass %), standard saline. The compiler estimates this is about 0.155 mol kg^{-1}.

Water+ Glucose (5 mass %). The compiler estimates this is about 0.29 mol kg^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:
The liquid/gas partition coefficients were obtained by a static headspace-gas chromatograph method.[1]

Source and Purity of Material:
(1) Sulfur hexafluoride. Gas chromatography gave a purity of better than 99% purity.
(2) Nothing specified.

Estimated Error:
See standard deviations in Table above.

References:
[1]R. Guitart, A. Puigdemont, and M. Arboix, J. Chromatography **491**, 271–280 (1989).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-19-5]

Original Measurements:
E. K. Morczek, J. Chem. Eng Data **42**, 116–119 (1997).

Variables:
T/K=347.3–505.6
p_t /MPa=0.162–2.951

Prepared By:
H. L. Clever

Experimental Values

Temperature			Pressure			Mole Fraction			
(t/°C)	(T/K)	(T/T_c)	($p_{t/MPa}$)	(p_s /MPa)	Molality ($10^6 m_1$ /mol kg^{-1})	Liq $10^6 x_1$	Vap y_1	Henry Const. ln(k_H /MPa)	Distribution Coeff. ln B
74.1	347.3	0.5367	0.164	0.037	172	3.09	0.774	10.61	13.91
74.3	347.5	0.5370	0.165	0.037	178	3.21	0.775	10.58	13.89
74.3	347.5	0.5370	0.164	0.037	180	3.24	0.774	10.56	13.87
74.4	347.6	0.5372	0.162	0.038	174	3.13	0.765	10.57	13.85
99.2	372.4	0.5755	0.226	0.099	153	2.75	0.560	10.72	13.04
99.2	372.4	0.5755	0.224	0.099	157	2.84	0.556	10.68	13.00
99.2	372.4	0.5755	0.225	0.099	153	2.76	0.558	10.71	13.03
124.1	397.3	0.6140	0.350	0.226	167	3.00	0.350	10.61	12.10
124.3	397.5	0.6143	0.350	0.227	159	2.87	0.347	10.64	12.13
124.4	397.6	0.6144	0.558	0.228	421	7.59	0.587	10.65	12.14
124.5	397.7	0.6146	0.349	0.229	166	2.99	0.340	10.58	12.06
124.5	397.7	0.6146	0.555	0.229	402	7.25	0.582	10.68	12.17
124.5	397.7	0.6146	0.556	0.229	450	8.11	0.583	10.57	12.06
124.7	397.9	0.6149	0.559	0.230	405	7.30	0.584	10.68	12.17
124.8	398.0	0.6151	0.560	0.231	410	7.38	0.583	10.67	12.15
148.5	421.7	0.6517	0.553	0.457	159	2.87	0.169	10.39	11.17
148.6	421.8	0.6518	0.554	0.459	145	2.61	0.169	10.39	11.25
148.8	422.0	0.6521	0.556	0.461	145	2.79	0.166	10.41	11.18
152.2	425.4	0.6574	0.626	0.505	192	3.47	0.188	10.43	11.11
152.3	425.5	0.6576	0.626	0.506	191	3.43	0.186	10.48	11.11
152.5	425.7	0.6579	0.626	0.509	189	3.40	0.182	10.41	11.09
162.0	435.2	0.6752	0.970	0.650	594	10.70	0.320	10.26	10.69
162.2	435.4	0.6729	0.970	0.653	555	10.00	0.320	10.33	10.76
162.5	435.7	0.6733	0.978	0.658	524	9.45	0.317	10.39	10.80
178.5	451.7	0.6980	1.047	0.968	173	3.12	0.072	10.10	10.12
178.7	451.9	0.6984	1.050	0.972	167	3.01	0.070	10.12	10.13
178.8	452.0	0.6985	1.053	0.975	176	3.01	0.070	10.07	10.13
206.2	479.4	0.7408	1.858	1.764	274	4.94	0.046	0.044	9.19
206.3	479.5	0.7410	1.860	1.768	255	4.59	0.046	9.85	9.24
206.3	479.5	0.7410	1.857	1.768	249	4.48	0.044	9.84	9.23
231.8	505.0	0.7804	0.7813	2.888	220	3.97	0.019	9.60	8.47
232.2	505.4	0.7810	2.975	2.909	214	3.86	0.019	9.68	8.54
232.4	505.6	0.7813	2.983	2.920	236	4.25	0.019	9.53	8.39

The compiler added the Kelvin temperatures and the reduced temperatures using 647.096 for the SF_6 critical temperature. The author calculated the Henry's constant from: k_H /MPa$=[(y_1\phi_1 p_t)/x_1]\exp\{-v_1^{\infty}(p_t-p_s)/RT\}$.

The vapor phase mole fraction was calculated from: $(1-y_1)=[((1-x_1)f_s p_s)/\phi_2 p_t]\exp\{v_s(p_t-p_s)/RT\}$.

The dimensionless gas distribution coefficient, B, is defined as: $B=[y_1(1-x_1)]/[(1-y_1)x_1]$.

The distribution coefficients are best fitted to temperature by the equation ln B=26.4987–0.03609/(T/K).

The data from the present work were combined with the data of Ashton *et al.*[1] and of Cosgrove and Walkley[2] using the EOS of Peng-Robinson to obtain the empirical equation:

$$\ln(k_H/\mathrm{MPa})=\ln(p_s/\mathrm{MPa})-14.8637/T^*+2.1337(1-T^*)^{0.355}/T^*-18.82(T^*)^{-0.41}\exp(1-T^*)$$

where T^* is the reduced temperature, $(T_1/\mathrm{K})/(T_{c,1}/\mathrm{K})$.

Smoothed values from the equation at 25 degree intervals from 298.15 K to 503.15 K are given below.

t/°C	T/K	ln(p_s /MPa)	ln(k_H /MPa)	ln B
25	298.15	−5.754	10.04	15.74
50	323.15	−4.394	10.46	14.84
75	348.15	−3.255	10.46	13.93
100	373.15	−2.289	10.68	13.93
125	398.15	−1.460	10.60	12.13
150	423.15	−0.742	10.43	11.23
175	448.15	−0.114	10.21	10.32
200	473.15	0.441	9.94	9.42
225	498.15	0.936	9.65	8.52
230	498.15	1.029	9.59	8.34

Symbols: p_t , p_s total pressure and pure water vapor pressure; x_1 , y_1 liquid and vapor SF_6 mole fractions; v^{∞}, v_s SF_6 partial mol volume at infinite dilution and H_2O pure liquid molal volume at saturation; ϕ_1 , ϕ_2 , ϕ_s SF_6 gas phase fugacity, H_2O gas phase fugacity and pure H_2O fugacity at saturation, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
A 100 cm^3 capacity stainless steel autoclave was filled with about 70 cm^3 degassed distilled water. The headspace was evacuated and then filled with SF_6 to a total pressure of less than 0.2 MPa at room temperature. The autoclave was heated in a rocking furnace. Temperature was measured with a thermocouple and total pressure measured with a pressure transducer. The system was equilibrated over night at a set temperature. Three samples were taken at 2 h intervals from the saturated liquid phase into a 50 μL gas tight syringe. The samples were analyzed by gas chromatography. The sample was stripped and diluted with an argon-methane mixture. The limit of detection was 1×10^{-17} mol SF_6 . More details are in the paper.

Source and Purity of Materials:
(1) Sulfar hexafluoride. Montefluos. Stated to be >99.97 mass %.
(2) Water. Distilled.

Estimated Error:
δT/K= ±0.2.
δp_t /kPa= ±12.
$\delta k_H/k_H$= ±0.10 at 348 K increasing to 0.20–0.30 above 473 K (authors).

References:
[1]J. T. Ashton, R. A. Dawe, K. W. Miller, E. B. Smith, and B. J. Stickings, J. Chem. Soc. **1968A**, 1793.
[2]B. A. Cosgrove and J. Walkley, J. Chromatogr. **161**, 216 (1981).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. L. Bullister, D. P. Wisegarver, and F. A. Menzia, Deep-Sea Research **I49**, 175–187 (2002).

Variables:
T/K = 273.33–312.87

Prepared By:
H. L. Clever

Experimental Data

t/°C	T/K	Solubility Coefficient ($10^3K'$/mol L^{-1} atm^{-1})	Mol Fraction at 1 atm 10^6x_1	Ostwald Coefficient (L/cm^3 cm^{-3})
0.18	273.33	0.61935	11.16	0.0139
0.25	273.40	0.61231	11.03	0.0137
0.28	273.43	0.60759	10.95	0.0136
0.38	273.53	0.61575	11.09	0.0136
10.27	283.42	0.39058	7.039	0.00908
10.32	283.47	0.39351	7.091	0.00915
10.34	283.49	0.39093	7.045	0.00909
10.36	283.41	0.38588	6.954	0.00898
10.40	283.55	0.39451	7.110	0.00918
20.01	293.16	0.27614	4.984	0.00664
20.01	293.16	0.27614	4.984	0.00648
20.06	293.21	0.27100	4.891	0.00652
20.17	293.32	0.26939	4.862	0.00648
30.82	303.97	0.19841	3.591	0.00495
31.27	304.42	0.19504	3.530	0.00487
31.38	304.53	0.19581	3.545	0.00489
31.48	304.63	0.19350	3.454	0.00484
32.16	305.31	0.19238	3.483	0.00482
39.09	312.24	0.16287	2.955	0.00417
39.11	312.26	0.15630	2.837	0.00401
39.11	312.26	0.16299	2.958	0.00418
39.38	312.53	0.15812	2.870	0.00406
39.52	312.67	0.15960	2.897	0.00409
39.63	312.78	0.15881	2.870	0.00408
39.72	312.87	0.15687	2.848	0.00403

The compiler added the Kelvin temperatures and calculated the mole fraction and Ostwald coefficients.

The authors fitted the data for the water and the seawater to the integrated van't Hoff equation and the logarithmic Sechenow salinity dependence to express K' as a function of temperature and salinity. The equations for molality and concentration forms are:

$$\ln(K'/\text{mol kg}^{-1}\ \text{atm}^{-1}) = -98.7264 + 140.803((T/\text{K})/100) + 38.8746\ \ln((T/\text{K})/100) + S[0.0268695 - 0.0334407((T/\text{K})/100) + 0.0070843((T/\text{K})/100)^2] \text{ and}$$

$$\ln(K'/\text{mol L}^{-1}\ \text{atm}^{-1}) = -96.5975 + 139.883((T/\text{K})/100) + 37.8193\ \ln((T/\text{K})/100) + S[0.0310693 - 0.0356385((T/\text{K}/100) + 0.00743254((T/\text{K})/100)^2].$$

S is the salinity. With $S=0$ the equations give the solubility in water. The equations fit the experimental data with a standard error of 1.20%.

Auxiliary Information

Method/Apparatus/Procedure:
The SF_6 in water and seawater at saturation was determined by a purge and trap electron capture/gas chromatography technique. See paper for details.

See the SF_6+seawater data sheet for this paper for the rest of the data from this paper.

Source and Purity of Material:
(1) Sulfur hexafluoride. Not specified.
(2) Water. Deionized. Taken from Millipore® Milli R015 system.

Estimated Error:
δT/K = ±0.05.
$\delta p_1/p_1$ = ±0.005.
$\delta K'/K'$ = ±0.01.

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Seawater

Original Measurements:
J. L. Bullister, D. P. Wisegarver, and F. A. Menzia Deep-Sea Research **I 49**, 175–187 (2002).

Variables:
T/K = 272.47–313.01

Prepared By:
H. L. Clever and M. Salomon

Experimental Data

Distribution Coefft/°C	T/K	Salinity* (S/g kg^{-1})	Solubility Coefficient** ($10^3K'$/mol L^{-1} atm^{-1})	Ostwald Coefficient (L/cm^3 cm^{-3})
−0.68	272.47	39.42	0.42080	0.00941
−0.46	272.69	39.42	0.41492	0.00928
−0.40	272.75	39.42	0.41489	0.00929
−0.38	272.77	39.42	0.411493	0.00929
−0.36	272.79	39.42	0.41017	0.00918
9.94	283.09	39.42	0.26192	0.00608
10.01	283.16	39.42	0.25970	0.00603
10.19	283.34	39.42	0.26006	0.00605
10.44	283.59	39.42	0.26403	0.00614
10.56	283.71	39.42	0.25945	0.00604
10.67	283.82	39.42	0.26042	0.00607
30.29	303.44	39.42	0.14232	0.00354
30.38	303.53	39.42	0.14096	0.00351
30.38	303.53	39.42	0.14257	0.00355
39.33	312.48	39.42	0.12028	0.00308
39.43	312.58	39.42	0.12034	0.00309
39.43	312.58	39.42	0.11953	0.00307
19.82	292.97	39.73	0.18578	0.00447
19.90	293.05	39.73	0.18920	0.00455
20.01	293.16	39.73	0.19009	0.00457
20.04	293.19	39.73	0.18859	0.00454
30.93	304.08	40.14	0.13764	0.00343
30.96	304.11	40.14	0.13803	0.00344
31.12	304.27	40.14	0.13913	0.00347
39.79	312.94	40.14	0.11341	0.00291
39.81	312.96	40.14	0.11363	0.00292
39.86	313.01	40.14	0.11544	0.00297

*The salinity, S, is defined as the mass in grams of dissolved inorganic matter in 1 kg of sea water after all Br^- and I^- have been replaced by the equivalent quantity of Cl^- and all HCO_3^- and CO_3^{2-} converted to oxide.
**See the SF_6+H_2O data sheet for author's equations for (K'/mol kg^{-1} atm^{-1}) and (K'/mol L^{-1} atm^{-1}).

Auxiliary Information

Method/Apparatus/Procedure:
The SF_6 in water and seawater at saturation was determined by a purge and trap electron capture/gas chromatography technique. See paper for details.
For more details see the SF_6+H_2O data sheet for this paper.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Not specified.
(2) Seawater. Obtained from the surface North Pacific Ocean subtropical gyre. Evaporated to a salinity of ≅39.4. Filtered through a 0.45 μm filter and poisoned with 0.5 mL sat. $HgCl_2$ per liter.

Estimated Error:
δT/K = ±0.05
$\delta p_1/p_1$ = ±0.005
$\delta K'/K'$ = ±0.01

Components:
(1) Sulfur fluoride or Sulfur hexafluoride; SF_6; [2551-62-4]
(2) Water-d_2; D_2O; [7789-20-0]

Original Measurements:
Rubin Battino, Wright State University, Dayton OH 45435
H. Lawrence Clever, Emory University, Atlanta, GA 30322 2002

Evaluation

An evaluation of the solubility of sulfur hexafluoride in heavy water at 0.101325 MPa between 278.15 K and 323.15 K

Two laboratories report the solubility of SF_6+D_2O. Cosgrove and Walkley[1] report nine values between 278.15 and 323.15 K. Scharlin and Battino[2] report five values between 288.21 and 318.15 K. At 288 K the workers values differ by 5.8%, at 298 K they differ by 2.4%, at 308 K they differ by 6.0% and at 318 K they differ by 0.8%. Scharlin and Battino have the larger value mole fractions at 288 and 298 and Cosgrove and Walkley have the larger values at 308 and 318 K. These differences are greater than the estimated experimental error of the workers. The data are classed as tentative.

In spite of these differences the combined data, excluding the 283 K value of Cosgrove and Walkley, when fit to the Clark, Glew, and Weiss equation reproduces the data with a maximum error of 3.4%. However the thermodynamic values calculated from the equation fall outside the norm and indicate a problem with these data. The CGW equation is:

$$\ln x_1 = -209.5271 + 294.3455/(T/100\ \mathrm{K}) + 90.2205 \ln(T/100\ \mathrm{K})$$

with $r^2 = 0.9965$ and the standard error of estimate 0.0230. The equation predicts a minimum in the solubility at 326 K (see Table 8).

Only a few of the values of the thermodynamic changes are given because they do not fit the pattern normally observed. The enthalpy and entropy change much more with temperature and the heat capacity is much larger than normally observed.

References

[1]B. A. Cosgrove and J. Walkley, J. Chromatogr. **216**, 161–167 (1981).
[2]P. Scharlin and R. Battino, J. Solution Chemistry **21**, 67–91 (1992).

TABLE 8. The tentative mole fraction solubility at a partial pressure of 0.101325 MPa, Ostwald coefficient and thermodynamic changes of enthalpy, entropy and heat capacity for the solution process at five degree intervals between 278.15 K and 323.15 K as calculated from the CGW equation above.

T/K	$10^6 x_1$	Ostwald, Coefficient ($10^2 L$/cm^3 cm^{-3})	$\Delta_{sln}H^o_1$ /kJ mol^{-1}	$\Delta_{sln}S^o_1$ /J K^{-1} mol^{-1}	$\Delta_{sln}C_p{}^o_1$ /J K^{-1} mol^{-1}
278.15	11.086	1.404	−36.08	−223	750
283.15	8.537	1.101	—	—	750
288.15	6.709	0.881	—	—	750
293.15	5.639	0.752	—	—	750
298.15	4.815	0.653	−21.08	−172	750
303.15	4.237	0.583	—	—	750
308.15	3.835	0.536	—	—	750
313.15	3.565	0.505	—	—	750
318.15	3.398	0.488	—	—	750
323.15	3.315	0.484	−2.33	−112	750

Components:
(1) Sulfur hexafluoride; SF_6; [2551-62-4]
(2) Water-d_2; (deuterium oxide); D_2O; [7789-20-0]

Original Measurements:
P. Scharlin and R. Battino, J. Solution Chem. **21**, 67–91 (1992).

Variables:
T/K = 288.15–318.15
p_1 /kPa = 101.325

Prepared By:
Pirketta Scharlin

Experimental Values

Ostwald coefficient and mole fraction of sulfur hexafluoride dissolved in deuterium oxide at 288–318 K and partial pressure of 101.325 kPa

T/K	$10^2 L$ [a,b]	$10^5 x_1$ [c,b]	$10^5 x_1$ [d]
288.15	—	—	0.6977
288.21	0.8894	0.6902	0.6958
297.99	0.6599	0.4950	0.4844
298.15	—	—	0.4821
308.14	0.5103	0.3708	0.3813
308.14	0.5143	0.3737	0.3813
308.15	—	—	0.3812
318.15	0.4845	0.3419	0.3394

[a]L = Ostwald coefficient [cm^3 cm^{-3}].
[b]Experimental value.
[c]x_1 = mole fraction of sulfur hexafluoride (corrected for nonideality).
[d]Smoothed value; calculated from the smoothing equation $\ln x_1 = -234.132 + 330.059/(T/100\ \mathrm{K}) + 101.780 \ln(T/100\ \mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus was based on a design of Ben-Naim and Baer,[1] which had been improved by modifications described in detail in Tominaga *et al.*[2] After degassing,[3] the solvent was transferred under its own vapor pressure into the evacuated mixing chamber. The gas buret was evacuated and the system filled with the solvent-saturated gas to a total pressure of about 1 atm. The computer program controlling the apparatus read the pressure of the system, which was tracked during the measurement. When the reading was stable, the pressure was adjusted to 1 atm and the corresponding pressure transducer reading became the setpoint for pressure control. After pre-equilibration, the initial volume of solvent was determined using a precision cathetometer. The dissolution was initiated by high-speed stirring of the solvent. After the system had reached equilibrium, stirring was stopped and the final volume of solvent was recorded. Gas volume was determined by a computer counting the number of steps a stepping motor used to drive a close-fitting stainless steel or teflon piston with two O-ring seals through a Fisher and Porter precision bore tube.

Source and Purity of Material:
(1) Airco, purity 99.8 mole %.
(2) Aldrich, 99.8 mole %. Degassed.

Estimated Error:
δT/K = 0.03
$\delta p/p = \pm 0.2\%$
$\delta L/L = \pm 1.0\%$

References:
[1]A Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6; [2551-62-4]
(2) Water-d_2; H_2O; [7789-20-0]

Original Measurements:

B. A. Cosgrove and J. Walkley, J. Chromatogr. **216**, 161–167 (1981).

Variables:

T/K = 278.15–323.15
p_1 /kPa = 101.325

Prepared By:

H. L. Clever

Experimental Values

Mole fraction solubility of sulfur hexafluoride in water from 278.15 K to 323.15 K at 1 atm (101.325 kPa) partial pressure

T/K	$10^4 x_1$
278.15	0.1106
283.15	0.17813
288.15	0.06505
293.15	0.05465
298.15	0.04829
303.15	0.04280
308.15	0.03960
313.15	0.03584
323.15	0.03311

Auxiliary Information

Method/Apparatus/Procedure:

A 20 mL volume of degassed (sublimation technique) solvent is transferred to a previously evacuated (10^{-4} mmHg) saturation cell immersed in an insulated, controlled (±0.01 K) water bath. The gas is dispersed through the constantly stirred solution at 1 atm by a coarse, fritted glass disc. Saturation is obtained within a few hours. Prior to analysis the solution is allowed to sit under 1 atm gas pressure for 1 h.
A saturated solution is withdrawn from the cell using a greaseless, gas tight Gilmont syringe of 2.500±0.001 mL volume. A 0.250 mL sample is injected to "wet" the frit. It is tripped and then four 0.500 mL samples are injected sequentially into the frit of the gas chromatograph. The stripped gas is dried before entering the column. The gas is analyzed on a dual filament conductivity detector. Calibrations with pure gas are made dry before and wet after each series of runs.

Source and Purity of Materials:

(1) Sulfur hexafluoride. Nothing specified.
(2) Water-d_2. Nothing specified.

Estimated Error:

δT/k = ±0.01
$\delta x_1 / x_1$ = ±0.015 (Estimate of compiler).

Components:

(1) Sulfur fluoride or Sulfur hexafluoride; SF_6; [2551-62-4]
(2) Electrolytes
hydrochloric acid; HCl; [7647-01-0]
Ammonium chloride [12125-02-9]
N,N,N-Trimethyl methanaminium iodide [75-58-1]
N,N,N-Triethyl ethanaminium bromide [71-91-0]
Barium chloride [14832-88-6]
Lithium chloride [7447-41-8]
Sodium chloride [7647-14-5]
Sodium sulfate [7757-82-6]
Sodium nitrite [7632-00-0]
Potassium hydroxide [1310-58-3]
Potassium chloride [7447-40-7]
Potassium bromide [7558-40-7]
Potassium iodide [7681-11-0]
Potassium nitrate [7757-79-1]
(3) Water; H_2O; [7732-18-5]

Evaluators:

H. Lawrence Clever,
Emory University,
Atlanta, GA 30322.
2002

Evaluation

An evaluation of the solubility of sulfur hexafluoride in aqueous electrolyte solutions

The solubility of nonelectrolytes in aqueous and other electrolyte solutions has long been of interest. The solubility of some substances are enhanced by the presence of an electrolyte (salted in) but for many more substances the solubility decreases in the presence of an electrolyte over its value in the pure solvent (salts out). Sechenov[1] was among the first to make careful studies of the salt effect. He reported extensive data on the solubility of carbon dioxide gas in aqueous electrolyte solutions and he proposed a simple equation to express the results of these studies.

Sechenov proposed the salt effect parameter, k_{syz}, which is positive for salting out and negative for salting in. The parameter can be defined for various composition scales. A general form for the empirical Sechenov salt effect parameter is:

$$k_{syz} = (1/y_2)\log(z^\circ_1/z_1)$$

where z°_1 is the solubility of component 1, the gas, in the pure solvent, and z_1 is the gas solubility in the electrolyte solution of salt composition y_2. The salt composition y_2 may be any of the quantities c_2 /mol L^{-1}, m_2 /mol kg^{-1} x_2 (mole fraction), I_{m2} (ionic strength in molality), and I_{c2} (ionic strength in concentration). The gas solubility z may be expressed in any of the quantities c_1 /mol L^{-1}, m_1 /mol kg^{-1}, x_1 (mole fraction), α_1 (Bunsen coefficient), L_1 (Ostwald coefficient), and S_1 (Kunen coefficient). The five quantities for y and the six quantities for z give 30 definitions for k_{syz}. The ratios of z values are the same for $z = c_1$, α_1, and L_1 and for m_1 and S_1, respectively, leaving 15 distinct definitions. If z is the same, the definitions of k_{syz} are related through ten equations between the y quantities pairs of c_1, m_1, x_1, I_m, and I_c. The details of the relations among k_{ssc}, k_{smm}, and k_{sxx} are given in SDS Volume 10[2] and in the recent book on Experimental Determination of Solubility.[3] The equations involving ionic strength are to be used when than one salt is present.

The difference between some of these definitions is small, but in the most careful work it is important. At gas solubilities greater than 0.01 mole fraction other factors become important such as density of the solution and partial mole volume of the dissolved gas. Also corrections should be made for the nonideality of the gas.

A useful graphical test of salt effect data is to put the salt effect equation into the form:

$$\log z = \log z^\circ - k_{syz} y$$

and plot log z vs y. The slope will be the negative of the salt effect parameter. The salt effect parameter units will be the inverse of the y units.

There are a number of more sophisticated approaches to salt effects, however, the empirical Sechenov equation seems to be the simplest approach to summarize a large body of data. Clever and Batino[4] give a brief review of other approaches to salt effects. Extensions of the empirical Sechenov salt effect parameter are given by van Krevelen and Hoftizer[5] and by Weisenberger and Schumpe.[6]

The salt effect data are given in the order of the standard arrangement for inorganic substances used by the U.S. National Institute of Standards and Technology. The number before each system is the standard order number for the cation. The number in ( ) keeps count of the number of salts with that cation studied.

The salt effect data for sulfur hexafluoride is sparse. We find only four papers listing salt effect data and none of these papers appears to present data of high reliability. One paper made only two measurements on each system; the solubility in water and in a 1 molal salt solution; two papers present only data for very dilute systems and such data has been observed to often be questionable and the fourth paper presents data on the solubility of sulfur hexafluoride in water that is appreciably lower than solubility data of other workers which makes all of the data suspect. All data below are classed as tentative.

2(1) Sulfur hexafluoride + hydrochloric acid; HCl; [7647-01-0] + Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in one molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The Evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}^{-1} = 0.040 \quad \text{and} \quad k_{smx}/\text{kg mol}^{-1} = 0.055$$

18(1) Sulfur hexafluoride+Ammonium chloride [12125-02-09]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in one molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The Evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}^{-1}=0.090 \text{ and } k_{smx}/\text{kg mol}^{-1}=0.105.$$

18(2) Sulfur hexafluoride+N,N,N-Trimethyl methanaminium iodide [75-58-1]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in one molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The Evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}^{-1}=0.010 \text{ and } k_{sms}/\text{kg mol}=0.025.$$

18(3) Sulfur hexafluoride+N,N,N-Triethyl ethanaminium bromide [71-91-0]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in 1 molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The Evaluator calculated the k_{smx} value. The values at 298.15 K are

$$k_{smm}/\text{kg mol}^{-1}=0.010 \text{ and } k_{smx}/\text{kg mol}=0.025.$$

96(1) Sulfur hexafluoride+Barium chloride [14832-88-6]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in 1 molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}=0.195 \text{ and } k_{smx}/\text{kg mol}=0.217.$$

98(1) Sulfur hexafluoride+Lithium chloride [7447-41-8]

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in 1 model salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The Evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}^{-1}=0.145 \text{ and } k_{smx}/\text{kg mol}^{-1}=0.160.$$

99(1) Sulfur hexafluoride+Sodium chloride [7647-14-5]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in 1 molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The Evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}^{-1}=0.195 \text{ and } k_{smx}/\text{kg mol}^{-1}=0.210.$$

99(2) Sulfur hexafluoride+Sodium sulfate [7757-82-6]+Water

Morrison and Johstone[7] measured the solubility of solubility of sulfur hexafluoride in water and in 1 molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The Evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}^{-1}=0.295 \text{ and } k_{smx}/\text{kg mol}^{-1}=0.317.$$

99(3) Sulfur hexafluoride+Sodium nitrite [7632-00-0]+Water

Longo, Dilivoria-Papadopoulas, Power, Hill, and Forster[9] measured the Bunsen coefficient of sulfur hexafluoride in water and in 0.14 mol L^{-1} sodium nitrite at 310.15 K. The evaluator calculated the salt effect parameter. It is k_{scc} /L $\text{mol}^{-1}=0.106$.

100(1) Sulfur hexafluoride+Potassium hydroxide [1310-58-3]+Water

Shoor, Walker, and Gubbins[8] report the solubility of sulfur hexafluoride in water and in four concentrations of potassium hydroxide up to 31.6 wt % KOH at the four temperatures 298.15, 313.15, 333.15, and 353.15 K. For the KOH solutions they report the mode fraction SF_6 solubility ratio, x^o/x, rather than the mol fraction solubility. This should be an important definitive study, unfortunately, the solubility values in water are significantly smaller than the values of other workers. See the SF_6+H_2O evaluation earlier in this work. That cast doubt on the reliability of the salt effect parameters given below. They are classed as tentative, but use them with caution.

T/K	KOH mass % range	KOH mol L^{-1} range	Salt Effect Parameter (K_{scx} /L mol^{-1})
298.15	0.0, 5.00, 13.50, 23.00, 31.6	0.0, 0.92, 2.67, 5.00, 7,35	0.326
313.15	0.0, 5.00, 13.50, 23.00, 31.6	0.0, 0.92, 2.67, 5.00, 7,35	0.297
333.15	0.0, 5.00, 13.50, 23.00, 31.6	0.0, 0.92, 2.67, 5.00, 7,35	0.278
353.15	0.0, 5.00, 13.50, 23.00, 31.6	0.0, 0.92, 2.67, 5.00, 7,35	0.262

The concentration, mol L^{-1}, values are the 298.15 K values.

100(2) Sulfur hexafluoride+Potassium chloride [7447-40-7]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in 1 molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The evaluator calculated the k_{smx} value. The values at 298.15 K are: k_{smm} /kg $\text{mol}^{-1}=0.165$ and k_{smx} /kg $\text{mol}^{-1}=0.180$.

Smith, Porter, and Miller[10] measured the solubility of sulfur hexafluoride in water and in a dilute solution of 0.15 mol L^{-1}KCl +0.01 mol L^{-1}Tris-HCl+about 0.02 mol $L^{-1}Na(N_3)$ for a total concentration of 1-1 electrolyte of 0.18 mol L^{-1} at temperatures of 283.8 and 298.2 K and a pressure of 3.55 MPa. The evaluator calculated salt effect parameters of 0.28 and 0.23 at 283.6 and 298.2, respectively. The dilute solution, the mixture of electrolytes and the high pressure make the reliability of these numbers difficult to judge. Use with caution.

100(3) Sulfur hexafluoride+Potassium bromide [7558-40-7]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in 1 molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}^{-1}=0.160 \text{ and } k_{smx}/\text{kg mol}^{-1}=0.175.$$

100(4) Sulfur hexafluoride+Potassium iodide [7681-11-0]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in 1 molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The evaluator calculated the k_{smx} value. The values at 298.15 are:

$$k_{smm}/\text{kg mol}^{-1}=0.145 \text{ and } k_{smx}/\text{kg mol}^{-1}=0.160.$$

100(5) Sulfur hexafluoride+Potassium nitrate [7757-79-1]+Water

Morrison and Johstone[7] measured the solubility of sulfur hexafluoride in water and in 1 molal salt solution at one temperature. They reported only the solubility in water and the salt effect parameter, k_{smm}. The evaluator calculated the k_{smx} value. The values at 298.15 K are:

$$k_{smm}/\text{kg mol}^{-1}=0.120 \text{ and } k_{smx}/\text{kg mol}^{-1}=0.135.$$

References

[1]J. Sechenov, Z. Phys. Chem. Stoechiom. Verwandtschaftsl. **8**, 657–660 (1891).
[2]C. L. Young, R. Battino and H. L. Clever in R. Battino, Eds., *Nitrogen and Air*, IUPAC Solubility Data Series, Vol. 10 (Pergamon Press, Oxford, UK, 1982), pp. xvi–xvii; H. L. Clever, *ibid.*, pp. xxix–xxxvii.
[3]J. W. Lorimer, *Quantities, Units and Conversions* in G. Heftner and R. P. T. Tomkins, eds., *The Experimental Determination of Solubilities* (Wiley, New York, 2003), Introduction.
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[7]T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).
[8]S. K. Shoor, R. D. Walker, Jr. and K. E. Gubbins, J. Phys. Chem. **73**, 312–317 (1969).
[9]L. D. Longo, M. Delivoria-Papadoloulas, G. G. Power, E. P. Hill, and R. E. Forster, Am. J. Physiology **219**, 561–569 (1970).
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Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Hydrochloric acid; HCl; [7647-61-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).

Variables:
T/K = 298.15
p_1 /kPa = 101.325
m_2 /mol kg^{-1} = 0, 1.0

Prepared By:
H. L. Clever

Experimental Values

Temperature		Salt Effect Parameter	
(t/°C)	(T/K)	(k_{smm} /kg mol^{-1})	(k_{smx} /kg mol^{-1})
25	298.15	0.040	0.055

The salt effect parameter was calculated from two measurements, the solubility of SF_6 in water, $S°/cm^3(STP)kg^{-1}$, and the solubility of the gas in a 1.0 molal salt solution. Only the solubility values in water (see earlier data sheet) and the salt effect parameter values are given in the paper. The computer calculated the k_{smx} salt effect parameter.

Auxiliary Information

Procedure/Apparatus/Method:
The degassed water or electrolyte solution flows in a thin film down a glass absorption helix containing the sulfur hexafluoride gas and water vapor at a total pressure of 1 atm. The volume of gas absorbed is measured in an attached buret system. The solvent is also measured.[1]

Source and Purity of Materials:
(1) Sulfur hexafluoride. Imperial Chemical Industries, Ltd.
(2) Hydrochloric acid. Nothing specified.
(3) Water. Nothing specified.

Error Estimate:
δk_{smm} /kg mol^{-1} = ± 0.010 (authors).

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948); *ibid.*, 3819 (1952).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Barium chloride; $BaCl_2$; [10361-37-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).

Variables:
T/K = 298.15
p_1 /kPa = 101.325
m_2 /mol kg^{-1} = 0, 1.0

Prepared By:
H. L. Clever

Experimental Values

Temperature		Salt Effect Parameter	
(t/°C)	(T/K)	(k_{smm} /kg mol^{-1})	(k_{smx} /kg mol^{-1})
25	298.15	0.195	0.217

The salt effect parameter was calculated from two measurements, the solubility of sulfur hexafluoride in water, $S°/cm^3(STP)kg^{-1}$, and the solubility of the gas in a 1.0 molal salt solution. Only the solubility value in water (see earlier data sheet) and the salt effect parameter values are given in the paper. The compiler calculated the k_{smx} salt effect parameter.

Auxiliary Information

Procedure/Apparatus/Method:
The degassed water or electrolyte solution flows in a thin film down a glass absorption helix containing the sulfur hexafluoride gas and water vapor at a total pressure of 1 atm. The volume of gas absorbed in measured in an attached buret system. The solubility in the solvent was previously measured.[1]

Source and Purity of Materials:
(1) Sulfur hexafluoride. Imperial Chemical Industries, Ltd.
(2) Lithium chloride. Nothing specified.
(3) Water. Nothing specified.

Error Estimate:
δk_{smm} /kg mol^{-1} = ± 0.010 (authors).

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948); J. Chem. Soc. 3819 (1952).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Lithium chloride; LiCl; [7447-41-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).

Variables:
T/K = 298.15
p_1 /kPa = 101.325
m_2 /mol kg^{-1} = 0, 1.0

Prepared By:
H. L. Clever

Experimental Values

Temperature		Salt Effect Parameter	
(t/°C)	(T/K)	(k_{smm} /kg mol^{-1})	(k_{smx} /kg mol^{-1})
25	298.15	0.145	0.160

The salt effect parameter was calculated from two measurements, the solubility of sulfur hexafluoride in water, $S°$/cm^3(STP)kg^{-1}, and the solubility of the gas in a 1.0 molal salt solution. Only the solubility value in water (see earlier data sheet) and the salt effect parameter value are given in the paper. The computer calculated the k_{smx} salt effect parameter.

Auxiliary Information

Procedure/Apparatus/Method:
The degassed water or electrolyte solution flows in a thin film down a glass absorption helix containing the sulfur hexafluoride gas and water vapor at a total pressure of 1 atm. The volume of gas absorbed is measured in an attached buret system. The solvent is also measured.[1]

Source and Purity of Materials:
(1) Sulfur hexafluoride. Imperial Chemical Industries, Ltd.
(2) Lithium chloride. Nothing specified.
(3) Water. Nothing specified.

Error Estimate:
δk_{smm} /kg mol^{-1} = ± 0.010 (authors).

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948); J. Chem. Soc. 3819 (1952).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Sodium chloride; NaCl; [7647-14-5] or
(2) Sodium sulfate; Na_2SO_4 ; [7757-82-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).

Variables:
T/K = 298.15
p_1 /kPa = 101.325
m_2 /mol kg^{-1} = 0, 1.0

Prepared By:
H. L. Clever

Experimental Values

	Temperature		Salt Effect Parameter	
Salt	(t/°C)	(T/K)	(k_{smm} /kg mol^{-1})	(k_{smx} /kg mol^{-1})
Sodium chloride	25	298.15	0.195	0.210
Sodium sulfate	25	298.15	0.295	0.317

The salt effect parameter was calculated from two measurements, the solubility of sulfur hexafluoride in water, $S°$/cm^3(STP)kg^{-1}, and the solubility of the gas in a 1.0 molal salt solution. Only the solubility value in water (see earlier data sheet) and the salt effect parameter value are given in the paper. The computer calculated the k_{smx} salt effect parameter.

Auxiliary Information

Procedure/Apparatus/Method:
The degassed water or electrolyte solution flows in a thin film down a glass absorption helix containing the sulfur hexafluoride gas and water vapor at a total pressure of 1 atm. The volume of gas absorbed is measured in an attached buret system. The solvent is also measured.[1]

Source and Purity of Materials:
(1) Sulfur hexafluoride. Imperial Chemical Industries, Ltd.
(2) Sodium chloride. Nothing specified.
(2) Sodium sulfate. Nothing specified.
(3) Water. Nothing specified.

Error Estimate:
δk_{smm} /kg mol^{-1} = ± 0.010 (authors).

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948); J. Chem. Soc. 3819 (1952).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Ammonium chloride; NH_4Cl; [12125-02-9],
N,N,N-Trimethyl methanaminium iodide (tetramethyl ammonium iodide); $C_4H_{12}NI$; [75-58-1],
N,N,N-Triethylethanaminium bromide(tetraethyl ammonium bromide); $C_8H_{20}NBr$; [71-91-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).

Variables:

T/K = 298.15
p_1 /kPa = 101.325
m_2 /mol kg^{-1} = 0, 1.0

Prepared By:

H. L. Clever

Experimental Values

Salt	Temperature (t/°C)	Temperature (T/K)	Salt Effect Parameter (k_{smm} /kg mol^{-1})	Salt Effect Parameter (k_{smx} /kg mol^{-1})
Ammonium chloride	25	298.15	0.090	0.105
Tetramethyl ammonium iodide	25	298.15	0.010	0.025
Tetraethyl ammonium bromide	25	298.15	0.010	0.025

The salt effect parameter was calculated from two measurements, the solubility of sulfur hexafluoride in water, $S°$/cm^3(STP)kg^{-1}, and the solubility of the gas in a 1.0 molal salt solution. Only the solubility value in water (see earlier data sheet) and the salt effect parameter values are given in the paper. The compiler calculated the k_{smx} salt effect parameter.

Auxiliary Information

Procedure/Apparatus/Method:

The degassed water or electrolyte solution flows in a thin film down a glass absorption helix containing the sulfur hexafluoride gas and water vapor at a total pressure of 1 atm. The volume of gas absorbed is measured in an attached buret system. The solvent is also measured.[1]

Source and Purity of Materials:

(1) Sulfur hexafluoride. Imperial Chemical Industries, Ltd.
(2) Salts. Nothing specified.
(3) Water. Nothing specified.

Error Estimate:

δk_{smm} /kg mol^{-1} = ± 0.010 (authors).

References:

[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948); J. Chem. Soc. 3819 (1952).

Components:

(1) Sulfure fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Potassium salts
Potassium chloride; KCl; [7447-40-7]
Potassium bromide; KBr; [7558-02-3]
Potassium iodide; KI; [7681-11-0]
Potassium nitrate; KNO_3 ; [7757-79-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. 3655–3659 (1955).

Variables:

T/K = 298.15
p_1 /kPa = 01.325
m_2 /mol kg^{-1} = 0, 1.0

Prepared By:

H. L. Clever

Experimental Values

Salt	Temperature (t/°C)	Temperature (T/K)	Salt Effect Parameter (k_{smm} /kg mol^{-1})	Salt Effect Parameter (k_{smx} /kg mol^{-1})
Potassium chloride	25	298.15	0.165	0.180
Potassium bromide	25	298.15	0.160	0.175
Potassium iodide	25	298.15	0.145	0.160
Potassium nitrate	25	298.15	0.120	0.135

The salt effect parameter was calculated from two measurements, the solubility of sulfur hexafluoride in water, $S°$/cm^3(STP)kg^{-1}, and the solubility of the gas in a 1.0 molal salt solution. Only the solubility value in water (see earlier data sheet) and the salf effect parameter value are given in the paper. The compiler calculated the k_{smx} salt effect parameter.

Auxiliary Information

Procedure/Apparatus/Method:

The degassed water or electrolyte solution flows in a thin film down a glas absorption helix containing the sulfur hexafluoride gas and water vapor at a total presure of 1 atm. The volume of gas absorbed is measured in an attached buret system. The solvent is also measured.[1]

Source and Purity of Materials:

(1) Sulfur hexafluoride. Imperial Chemical Industries, Ltd.
(2) Potasium salts. Nothing specified.
(3) Water. Nothing specified.

Estimated Error:

δk_{smm} /kg mol^{-1} = ± 0.010 (authors).

References:

[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948); J. Chem. Soc. 3819 (1952).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Nitrous acid, sodium salt or sodium nitrite; $NaNO_2$; [7632-00-0]
Water; H_2O; [7732-18-5]

Original Measurements:
L. D. Longo, M. Delivoria-Papadopoulas, G. G. Power E. P. Hill, and R. E. Forster, Am. J. Physiology **219**, 561–569 (1970).

Variables:
T/K = 310.15

Prepared By:
C. L. Young and H. L. Clever

Experimental Data

T/K	c_2 /mol L^{-1}	Bunsen Coefficient [α/cm^3(STP)cm^{-3}]	Standard Deviation
310.15	0.0	0.00386	0.0001
310.15	0.14	0.00373	0.00006

The compiler calculated the Salt Parameter from: k_{scc} /L mol^{-1} = (1/(c_2 /mol L^{-1}))log($c_1°/c_1$)=0.10$_6$.

Auxiliary Information

Procedure/Apparatus/Method:
Liquid samples were equilibrated with gas and then the dissolved gas was stripped out under vacuum and measured in a manometric Van Slyke apparatus. Some details in Power.[1]
Two to 12 measurements were made for each value.

Source and Purity of Materials:
(1) Sulfur hexafluoride.
(2) Sodium nitrite.
(3) Water.
Nothing specified about components.

Estimated Error:
$\delta T/K = \pm 0.03$

References:
[1]G. G. Power, J. Appl. Physiology **24**, 468 (1968).

Components:
(1)Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) various media
Human blood and sheep placental tissue components
Water; H_2O; [7732-18-5]

Original Measurements:
L. D. Longo, M. Delivoria-Papadopoulas, G. G. Power, E. P. Hill, and R. E. Forster, Am. J. Physiology **219**, 561–569 (1970).

Variables:
T/K = 310.15

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

T/K	Solvent	Bunsen Coefficient [α/cm^3(STP)cm^3]	Standard Deviation
310.15	Water	0.00386	0.0001
310.15	Human Whole Blood	0.00671	0.00024
310.15	Plasma	0.00647	0.00044
310.15	Packed Erythrocytes	0.00734	0.00064
310.15	Sheep Placental Tissue	0.0078	0.0006

Two to 12 measurements were made for each system.

The values were corrected for the presence of 0.14 mol L^{-1} $NaNO_2$.
The human blood hematocrit was 47 vol %, the hemoglobin 15.7 g.

Auxiliary Information

Procedure/Apparatus/Method:
Liquid samples were equilibrated with gas and then the dissolved gas was stripped out under vacuum and measured in a manometric Van Slyke apparatus. Some details in Power.[1]
Each value is the average of from two to 12 measurements.

Source and Purity of Materials:
(1)Sulfur hexafluoride.
(2) Water.
Human blood and components.
Sheep placental tissue.
Nothing specified about components.

Estimated Error:
δT/K = $\pm$0.03

References:
[1]G. G. Power, J. Appl. Phsiology **24**, 468 (1968).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-2]
(2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$;[ ]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
A. M. Mainar, Dissertation, Universidad de Zaragoza, 2000.

Variables:
T/K = 298.15
p_1 /kPa = 101.33
x_2 = 0 – 1.0; x_3 = 1.0 – 0

Prepared By:
H. L. Clever

Experimental Values
Data at 298.15 K

Solvent mol fraction $C_2H_3F_3O/x_2$	Solvent Density (ρ/g cm^{-3})	Gibbs Energy of Solution ($\Delta G°_3$ /kJ mol^{-1})	Solubility mol Fraction $SF_6/10^4x_1$	Henry's Conant ln(K_H /Pa)
0	0.99707	30.58	0.0439	23.86
0.0276	1.04437	30.40	0.0471	23.78
0.0594	1.09952	29.00	0.0830	23.21
0.0993	1.13558	25.31	0.3685	21.72
0.1442	1.17640	22.94	0.9568	20.77
0.1920	0.21067	21.40	1.7810	20.15
0.2637	1.24949	19.55	3.753	19.40
0.3638	1.28771	17.99	7.058	18.77
0.4638	1.31471	16.68	11.97	18.24
0.6940	1.35420	14.61	27.52	17.4
1	1.38209	12.88	55.47	16.71

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent vapor saturated gas.

Source and Purity of Material:
(1) Sulfur hexafluoride. Air Liquide Espana. Stated to be 99.5 mol %.
(2) 2,2,2-Trifluoroethanol. Flurchem Ltd. Stated to be >99%.
(3) Water. Double distilled and deionized (Milli-Q).

Estimated Error:
δT/K = ±0.05 cell,
±0.2 burets;
$\delta x_1/x_1$ = ±0.007 (author).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-2]
(2) 1,1,1,3,3,3-Hexafluoropropanol-2; C_3HF_6O; [ ]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
A. M. Mainar, Dissertation, Universidad de Zaragoza, 2000.

Variables:
T/K = 298.15
p_1 /kPa = 101.33
x_2 = 0 – 1.0; x_3 = 1.0 – 0

Prepared By:
H. L. Clever

Experimental Data
Data at 298.15 K

$C_2H_3F_3O$ mol Fraction x_2	Solvent Density (ρ/g cm^{-3})	Gibbs Energy of Solution ($\Delta G°_3$ /kJ mol^{-1})	Solubility 10^4x_1	Henry's Constant ln(K_H /Pa)
0	0.99707	30.58	0.0439	23.86
0.0191	1.06502	29.52	0.0674	23.42
0.0418	1.13235	24.45	0.5183	21.38
0.0701	1.20046	21.81	1.509	20.31
0.1024	1.26213	20.16	2.939	19.65
0.1452	1.32515	18.77	5.150	19.09
0.1994	1.38381	17.52	8.505	18.58
0.2870	1.44783	15.96	16.00	17.95
0.4147	1.50423	14.27	31.66	17.27
0.6158	1.55329	12.46	65.72	16.54
0.8376	1.58493	11.19	109.6	16.54
1	1.60423	11.19	143.6	15.76

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent vapor saturated gas.

Source and Purity of Material:
(1) Sulfur hexafluoride. Air Liquide Espana. Stated to be 99.5 mol %.
(2) 1,1,1,3,3,3-Hexafluoropropanol-2. Flurchem Ltd. Stated to be >99%.
(3) Water. Double distilled and deionized (Milli-Q).

Estimated Error:
δT/K = ±0.05 cell, ±0.2 burets;
$\delta x_1/x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Pentane; C_2H_{12} ; [109-66-0]

Original Measurements:

I. Wichterle and Z. Wagner, Coll. Czech. Chem. Soc. **54**, 2863–2867 (1989).

Variables:

T/K = 319.15, 321.15, and 328.57
p_{tot} /MPa = 2.446 – 3.937

Prepared By:

H. L. Clever

Experimental Data

Temperature (T/K)	Total Pressure (P_{tot} /MPa)	Mole Fraction SF_6 Liquid, x_1	Mole Fraction SF_6 Vapor, y_1
319.15	2.446	0.4242	0.8243
319.15	3.316	0.7959	0.8942
319.15	3.500	0.8701	0.9223
319.15	3.592	0.9105	0.9453
319.15	3.671	0.9424	0.9616
319.15	3.707	0.9602	0.9700
319.15	3.741	0.9729	0.9774
319.15	3.750	0.9759	0.9800
319.15	3.783	0.990	0.990
321.15	3.596	0.8524	0.9070
321.15	3.726	0.9061	0.9288
321.15	3.773	0.9297	0.9389
321.15	3.787	0.9333	0.9412
321.15	3.794	0.9369	0.9416
321.15	3.802	0.947	0.947
328.57	3.845	0.7758	0.8429
328.57	3.893	0.7907	0.8437
328.57	3.927	0.8018	0.8359
328.57	3.930	0.8096	0.8342
328.57	3.932	0.8138	0.8335
328.57	3.933	0.8128	0.8281
328.57	3.937	0.822	0.822

Auxiliary Information

Method/Apparatus/Procedure:

The measurements were carried out in the high-pressure static cell described by Wagner and Wichterle[1] and Wagner and Berg.[2]

The critical temperature of SF_6 is T_{cr} = 318.67 K.

Measurements were made at temperatures of $T - T_{cr}$ = 0.48, 2.48 and 9.90 K.

In Table: pressure value is the critical pressure of the system.

Source and Purity of Materials:

(1) Sulfur hexafluoride. Nothing specified.
(2) Pentane. Nothing specified.

Estimated Error:

δT/K = ±0.01 (author's estimates)
δp/MPa = ±0.001
δx = ±0.0002

References:

[1]Z. Wagner and I. Wichterle, Fluid Phase Eq. **33**, 109 (1987).
[2]Z. Wagner and J. Berg, Fluid Phase Eq. (in press).

Components:

(1) Sulfur fluoride or sulfur hexalfuoride; SF_6 ; [2551-62-4]
(2) Alkanes (C_6 to C_{16})
Hexane; C_6H_{14} ; [110-54-3]
Heptane; C_7H_{16} ; [142-85-5]
Octane; C_8H_{18} ; [111-65-9]
Nonane; C_9H_{20} ; [111-84-2]
Decane; $C_{10}H_{22}$; [124-18-5]
Undecane; $C_{11}H_{24}$; [1120-21-4]
Dodecane; $C_{12}H_{26}$; [112-40-3]
Tridecane; $C_{13}H_{28}$; [629-50-5]
Tetradecane; $C_{14}H_{30}$; [629-59-4]
Pentadecane; $C_{15}H_{32}$; [629-62-9]
Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:

P. J. Hesse, R. Battino, P. Scharlin, and E. Wilhem, J. Chem. Eng. Data **41**, 195–201 (1996).

Variables:

T/K = 298.15
P_1 /MPa = 0.101325

Prepared By:

H. L. Clever

Experimental Data

Ostwald coefficient and Henry fugacity of sulfur hexafluoride at 298.15 K and a *total* pressure of 101 325 Pa. The sulfur hexafluoride mole fraction solubility at 298. 15 K and a *partial* pressure of 101 325 Pa

Alkane	Ostwald Coefficient/$L_{1,2}(T,p)$	Henry Fugacity/$(10^{-6}H_{1,2}T,p_{s,2})$/Pa	10^4x_1
Hexane	1.971	9.280	107.7
Heptane	1.687	9.720	102.7
Octane	1.450	10.22	97.68
Nonane	1.226	10.66	93.63
Decane	1.098	11.28	88.49
Undecane	0.9731	11.75	84.96
Dodecane	0.8834	12.02	83.06
Tridecane	0.8086	12.25	81.45
Tetradecane	0.7644	12.15	82.13
Pentadecane	0.7191	12.16	82.10
Hexadecane	0.6787	12.17	82.05

The refractive indices of the liquid alkanes were measured. The values were in good agreement with reliable literature values. The purity of the solvents were measured by gas chromatography and found to be greater than 99 mol % in all cases. The liquid alkanes were stored in brown glass bottles. Prior to the actual solubility measurements they were degassed by the method of Battino *et al.*[2] and transferred into the apparatus under their own vapor pressure.

Alkane properties listed and used by the authors are given on the following page. See paper for references. The numbers in the columns correspond to the following:

1 = Alkane; 2 = Vapor pressure, $p_{s,2}$ /Pa; 3 = Density, $10^{-3}\rho_2{}^L/(\mathrm{kg\ m^{-3}})$; 4 = Isobaric expansivity, $10^3\alpha_{p,2}{}^L/\mathrm{K}^{-1}$
5 = Isothermal compressibility, $10^{12}\beta_{T,2}{}^L/\mathrm{Pa}^{-1}$; 6 = Internal pressure, $10^{-6}\Pi_2{}^L$/Pa; 7 = Acentric factor, ω_2
8 = Critical temperature, $T_{c,2}$ /K; 9 = Critical pressure, $10^{-6}p_{c,2}$ /Pa;
10 = Critical molar volume, $10^6V_{c,2}$ /($\mathrm{m^3\ mol^{-1}}$).

Alkane properties listed and used by the authors.

1	2	3	4	5	6	7	8	9	10
Hexane	20179	0.6549	1.387	1669	247.8	0.299	507.90	3.035	369.9
Heptane	6104	0.6795	1.252	1438	259.6	0.350	540.15	2.735	430.1
Octane	1875	0.6985	1.155	1282	268.6	0.397	568.95	2.490	492.4
Nonane	584	0.7138	1.088	1175	276.1	0.443	594.90	2.290	555.2
Decane	183	0.7264	1.042	1094	284.0	0.490	617.65	2.105	624.1
Undecane	58	0.7365	1.004	1031	290.3	0.533	638.85	1.955	688.6
Dodecane	19	0.7452	0.976	988	294.5	0.573	658.65	1.830	753.7
Tridecane	6	0.7527	0.951	948	299.1	0.618	676	1.710	823.1
Tetradecane	2	0.7592	0.929	910	304.4	0.654	693	1.610	893.7
Pentadecane	>1	0.7649	0.911	882	308.0	0.696	708	1.515	965.5
Hexadecane	>1	0.7699	0.895	857	311.4	0.737	722	1.435	1034.0

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were measured with a Ben-Naim/Baer type apparatus as modified by the Tominanga *et al.*[1] The apparatus has four equilibration cells of ~26, 65, 380, and 1650 cm^3 volume for different ranges of Ostwald coefficients. The equilibration vessels and the gas burets were calibrated with doubly distilled water, and the respective volumes are known to ± 0.01 cm^3. The total pressure was determined with a pressure transducer. The entire apparatus is in a large air thermostat controlled to better than ± 0.01 K. Temperatures were measured by a calibrated platinum resistance cell based on IPTS-68. Prior to measurement the solvents were degassed by the method of Battino *et al.*[2] and transferred under their own vapor pressure into the solubility apparatus.

Source and Purity of Materials:

(1) Sulfur hexafluoride. Airco. Minimum mole percent purity stated to be 99.8.
(2) Alkanes

Heptane; Philips Petroleum, >99 mol %
Octane; General Dynamics, >99 mol %
Nonane; Philips Petroleum, >99 mol %
Decane; Philips Petroleum, >99 mol %
Undecane; Philips Petroleum, >99 mol %
Dodecane; Philips Petroleum, >99 mol %
Tridecane; Alfa Products, >99 mol %
Tetradecane; Philips Petroleum, >99 mol %
Pentadecane; Alfa Products, >99 mol %
Hexadecane; Philips Petroleum, >99 mol %

Estimated Error:
δT/K = ± 0.1
$x_1 / x_1 = \pm 0.002$ (authors).

References:
[1]T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[2]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Heptane; C_7H_{16} ; [142-82-5]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 279.46–309.31
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	$10^2 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
6.31	279.46	1.273	2.00	2.05
16.00	289.15	1.119	1.74	1.84
25.08	298.23	1.007	1.55	1.69
33.16	309.31	0.9322	1.41	1.60

The complier calculabed the Bunsen and Ostwald coefficient values, assuming an ideal gas and Henry's laws behavior.
Smoothed data for use between 278.15 K and 309.31 K: $\ln x_1 = -7.6341 + 9.1069/(T/100\ \mathrm{K})$
The standard error about the regression line is 2.00×10^{-4}.

T/K	$10^2 x_1$
278.15	1.279
288.15	1.141
298.15	1.026
308.15	0.929

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liqud N_2, evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is scaled off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is strirred, equilbration is attained with 24 h.

Source and Purity of Materials:

(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be minimum purity of 99 mol %, further purified by sublimation.
(2) Heptane. Fisher Co. Spectroanalytical grade. Dried with Drierite and distilled.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.002$ (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Octane; C_8H_{18} ; [111-65-9]

Original Measurements:
R. J. Wilcock, R. Battino, W. F. Danforth, and E. Wilhelm, J. Chem. Thermodyn. **10**, 817–822 (1978).

Variables:
T/K = 283.25–313.39
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
283.25	11.30	1.573	1.631
298.21	93.80	1.283	1.401
313.39	79.44	1.068	1.225

The complier calcualted the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 283.15 K and 313.15 K: $\ln x_1 = -8.1485 + 10.3804/(T/100\ \mathrm{K})$
The standard error about the regression line is 1.86×10^{-5}.

T/K	$10^4 x_1$
283.15	113.1
293.15	99.8
298.15	94.0
303.15	88.8
313.15	79.6

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino, Evans, and Danforth.[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) Octane. Phillips Petroleum Co. Stated to be 99 mole %. Distilled, density at 298.15 K, ρ/g cm^{-3} = 0.6988.

Estimated Error:
δT/K = ±0.02
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Octane; C_8H_{18} ; [142-82-5]

Original Measurements:
E. Wilhelm and R. Battino, J. Chem, Thermodyn. **3**, 379–392 (1971).

Variables:
T/K = 297.56–308.50
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
297.56	96.8	1.33	1.452
297.60	96.2	1.34	1.461
308.50	85.4	1.17	1.317
308.50	85.9	1.18	1.325

The complier calcualted the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 297.56 K and 308.50 K: $\ln x_1 = -8.0107 + 10.0281/(T/100\ \mathrm{K})$
The standard error about the regression line is 3.74×10^{-5}.

T/K	$10^4 x_1$
298.15	95.9
303.15	90.7
313.15	86.0

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Matheson Co., Inc. Purity better than 99 mol %.
(2) Octane. Phillips Petroleum Co. Fractionally distilled through a packed vacuum jacketed 1 m column at a reflux ratio of 20 or better. ρ/g cm^{-3} = 0.6988.

Estimated Error:
$\delta L/L$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Hexane; C_6H_{14} ; [110-54-3] or 2,2,4-Trimetylpentane or isooctane; C_8H_{18} ; [540-84-1]

Original Measurements:
L. E. W. Horsman-van den Dool and J. W. Warman, Interuniversity Reactor Institute (IRI)-Report, 134-81-01

Variables:
T/K = 291.1, 296.7
P_1 /kPa = not given.

Prepared By:
H. L. Clever

Experimental Data

Solvent (temperature)	Ostwald Coefficient (L/cm^3 cm^{-3})	Number of Runs
Hexane (17.9 °C, 291.1 K)	2.24	1
2,2,4-Trimethylpentane (23.5 °C, 296.7 K	2.14	1

Auxiliary Information

Method/Apparatus/Procedure:
A cylindrical glass container of approximately 15 cm^3 volume is filled with solvent and closed with a half-hole septum. An amount of gaseous solute is added to the container. The closed container is shaked for 30 min. Samples of both the vapor and liquid phases are taken in calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.
The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 20 cm Porapack Q column is used for the separation.

Source and Purity of Material:
(1) Sulfur hexafluoride. Baker Chemical Co. Instrument grade, 99.99%. Used as received.
(2) Hexane and 2,2,4-Trimethylpentane. Both Merck, Uvasol Spektoskopie Grade. Impurities, which give the same retention time as the gas, are removed before the experiment by adsorption or distillation.

Estimated Error:
$\delta L/L = \pm 0.05$

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 2,2,4-Trimethylpentane or isooctane; C_6H_{18} ; [540-84-1]

Original Measurements:
Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331–335 (1961).

Variables:
T/K = 282.84–303.27
p_1 /kPa = 101.325

Prepared By:
M. E. Derrick and H. L. Clever

Experimental Data

t/°C	T/K	$10^2 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
9.69	282.84	1.852	2.59	2.68
18.51	291.66	1.678	2.32	2.68
24.51	297.66	1.5435	2.12	2.31
25.00	298.15	1.535	2.10	2.29
30.12	303.27	1.428	1.94	2.15

The 298.15 K value may be a smoothed value of the authors. The compilers calcualted the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 282.84 K and 303.27 K: $\ln x_1 = -7.8229 + 10.8636/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.46×10^{-4}.

T/K	$10^2 x_1$
283.15	1.857
288.15	1.737
293.15	1.629
298.15	1.531
303.15	1.442

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consists of a gas measuring buret, an absorption pipet and a reservoir for the solvent. The buret is thermostated at 25 °C, the pipet from any temperature between 5 °C and 30 °C. The pipet contains a magnetic stirring bar. The pure solvent is degassed by freezing with liqud N_2 , evacuating, then boiling with a heat lamp. The process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. The solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by Hg. Its volume is the difference between the capacity of the pipet and the volume of Hg that confines it. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements in the buret before and after introduction of the gas into the buret. With stirring, equilibration is attained in 24 h.

Source and Purity of Material:
(1) Surlfur hexafluoride. Matheson Co., Inc. Stated to be 99%. Purified further by multiple trap sublimation at dry ice alcohol temperatures.
(2) Isooctane. Phillips Petroleum Co. Pure grade. Dried over $Mg(ClO_4)_2$ and fractionated through a 15 plate column at a reflux ratio of 20:1. Boiling point = 99.1 °C.

Estimated Error:
δT/K = 0.02
$\delta x_1 / x_1 = 0.003$

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 2,2,4-Trimethylpentane; C_8H_{14} ; [540-84-1]

Original Measurements:
P. J. Hesse, R. Battino, P. Scharlin, and E. Wilhelm, J. Chem Thermodyn. **31**, 1175–1181 (1999).

Variables:
T/K = 298.15
p_1 /Pa = 101,325

Prepared By:
H. L. Clever

Experimental Data

Temperature (T/K)	Ostwald Coefficient ($L_{1,2}$/cm^3 cm^{-1})	Henry's Constant $10^{-6}H_{1,2}(T,p_{s,2})$/Pa	Solubility 10^4x_1
298.15	2.219	6.578	151.7

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was measured with a Ben-Naim Baer type apparatus as modified by Tominaga *et al.*[1] The apparatus had several equilibration chambers from 26 to 1650 cm^3 to cover a large range of Ostwald Coefficient values. The equilibration vessels and the gas burets were calibrated with double distilled water and the volumes are known to ±0.01 cm^3. Gas volumes were determined using a microprocessor that counted the number of steps on a stepping motor which advanced a precision screw which moved in a close-fitting piston. The volumes were determined to a few parts per thousand. The pressure was measured with a pressure transducer and was kept nulled to within one part per thousand. A typical dissolution time to a stable equilibrium point was about 3 h. Prior to the measurement the solvent was degassed by the method of Battino *et al.*[2] and transferred under its own vapor pressure into the solubility apparatus.

Source and Purity of Material:
(1) Sulfur hexafluoride. Matheson or Airco. Used as received. Stated to be of 0.997 minimum mass fraction purity.
(2) 2,2,4-Trimethylpentane or isooctane. Philips Petroleum. R.I. (n_D) agreed well with accepted literature vaule. GLC found a purity of >0.99 mass fraction.

Estimated Error:
δT/K = ±0.05
$\delta p/p$ = ±0.001
$\delta x_1/x_1$ = ±0.002
Author's estimates.

References:
[1]T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[2]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Decane; $C_{10}H_{22}$; [124-18-5]

Original Measurements:
R. J. Wilcock, R. Battino, W. F. Danforth, and E. Wilhelm, J. Chem. Thermodyn. **10**, 817–822 (1978).

Variables:
T/K = 282.61–313.45
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

T/K	10^4x_1	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
282.61	105.0	1.217	1.259
298.12	87.36	0.997	1.088
313.45	75.37	0.847	0.972

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 283.15 K and 313.15 K: $\ln x_1 = -7.9322 + 9.5329/(T/100\ \text{K})$.
The standard error about the regression line is 6.20×10^{-5}.

T/K	10^4x_1
283.15	104.1
293.15	92.8
298.15	87.8
303.15	83.3
313.15	75.4

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) Decane. Phillips Petroleum Co. Stated to be 99 mole %. Distilled, density at 298.15 K, ρ/g cm^{-3} = 0.7264.

Estimated Error:
δT/K = ±0.02
δp/mmHg = ±0.5
$\delta x_1/x_1$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Cyclopentane; C_5H_{10} ; [287-92-3] or
Cyclooctane; C_8H_{16} ; [292-64-8]

Original Measurements:
L. E. W. Horsman-van den Dool and J. W. Warman, Interuniversity Reactor Institute (IRI)-Report 34-81-01.

Variables:
T/K = 294.3, 298.2 and 299.6
P_1 /kPa = not given.

Prepared By:
H. L. Clever

Experimental Data

Solvent (temperature)	Ostwald Coefficient (L/cm^3 cm^{-3})	Number of Runs
Cyclopentane (26.4 °C, 299.6 K)	1.58	3
Cyclooctane (21.1 °C, 294.3 K)	0.64	1
Cyclooctane (25.0 °C, 298.2 K)	0.62	1

Auxiliary Information

Method/Apparatus/Procedure:
A cylindrical glass container of approximately 15 cm^3 volume is filled with solvent and closed with a half-hole septum. An amount of gaseous solute is added to the container. The closed container is shaken for 30 min. Samples of both the vapor and liquid phases are taken in calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.
The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 20 cm Porapack Q column is used for the separation.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Baker Chemical Co. Instrument Grade, 99.9 percent. Used as received.
(2) Cyclopentane. Merck. Uvasol spektroskopie grade.
(2) Cyclooctane. Fluka purum grade. Impurities which give the same retention time as the solute gas were removed by absorption or distillation.

Estimated Error:
$\delta L/L = \pm 0.05$

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 280.29–306.77
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

t/°C	T/K	$10^3 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
7.14	280.29	6.288	1.33	1.36
17.79	290.94	5.714	1.19	1.27
26.78	299.93	5.389	1.11	1.22
33.62	306.77	5.055	1.04	1.17

The compiler calculated the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 278.15 K and 308.15 K: $\ln x_1 = -7.5411 + 6.9269/(T/100\ \mathrm{K})$.
The standard error about the regression line is 3.95×10^{-5}.

T/K	$10^3 x_1$
278.15	6.405
288.15	5.874
298.15	5.419
308.15	5.026

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2 , evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilbration is attained within 24 h.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be minimum purity of 99 mol %, further purified by sublimation.
(2) Cyclohexane. Eastman Organic Chemical Co. Analytical Reagent. Dried with Drierite and distilled.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.002$ (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6; [2551-62-4]
(2) Cyclohexane; C_6H_{12}; [110-82-7] or
Methylcyclohexane; C_7H_{14}; [108-87-2]

Original Measurements:
L. E. W. Horsman-van den Dool and J. W. Warman, Interuniversity Reactor Institute (IRI)-Report 134-81-01.

Variables:
T/K = 292.8–299.2
p_1 /kPa = not given.

Prepared By:
H. L. Clever

Experimental Data

Solvent	t/°C	T/K	Ostwald Coefficient (L/cm^3 cm^{-3})	Number of Runs
Cyclohexane	19.6	292.8	1.24	2
Cyclohexane	23.6	296.8	1.18	5
Cyclohexane	26.0	299.2	1.17	5
Methylcyclohexane	23.2	296.4	1.34	2

Auxiliary Information

Method/Apparatus/Procedure:
A cylindrical glass container of approximately 15 cm^3 volume is filled with solvent and closed with a half-hole septum. An amount of gaseous solute is added to the container. The closed container is shaken for 30 min. Samples of both the vapor and liquid phases are taken in calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.
The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 20 cm Porapack Q column is used for the separation.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Baker Chemical Co. Instrument Grade, 99.9%. Used as received.
(2) Cyclohexane. Merck and Co.
Uvasol spektroskopie grade.
(2) Methylcyclohexane. Fluka. UV-Spektoskopie grade. Impurities which give the same retention time as the solute gas are removed by absorption or distillation.

Estimated Error:
$\delta L/L = \pm 0.05$

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6; [2551-62-4]
(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 281.06–307.47
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

t/°C	T/K	$10^3 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
7.91	281.06	8.415	1.51	1.55
14.77	287.92	7.749	1.38	1.45
26.89	300.04	7.044	1.24	1.36
34.82	307.47	6.394	1.11	1.25

The compiler calculated the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 281.06 K and 307.47 K: $\ln x_1 = -7.9579 + 8.9301/(T/100\ \mathrm{K})$.
The standard error about the regression line is 3.92×10^{-5}.

T/K	$10^3 x_1$
283.15	8.196
288.15	7.760
298.15	6.994
308.15	6.346

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2, evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilbration is attained within 24 h.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be minimum purity of 99 mol %, further purified by sublimation.
(2) Methylcyclohexane. Eastman Organic Chemical Co. Analytical Reagent. Dried with Drierite and distilled.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.002$ (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) *cis*-1,2-Dimethylcyclohexane; C_8H_{16} ; [2207-01-4]

Original Measurements:
E. B. Geller, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **8**, 197–202 (1976).

Variables:
T/K = 298.12, 312.93
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
298.12	62.61	0.997	1.088
312.93	52.50	0.823	0.943

The Bunsen coefficients were calculated by the compiler, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 298.12 K and 312.93 K: $\ln x_1 = -8.7968 + 11.1005/(T/100\ \mathrm{K})$.

T/K	$10^4 x_1$
298.15	62.59
308.15	55.47

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino, Evans, and Danforth.[2] The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm.[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) *cis*-1,2-Dimethylcyclohexane. Chemical Samples Co. Fractionally distilled and stored in the dark. Refractive index (NaD, 298.15 K) 1.4337.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) trans-1,2-Dimethylcyclohexane; C_8H_{16} ; [6876-23-9]

Original Measurements:
E. B. Geller, R. Battino and E. Wilhelm J. Chem. Thermodyn. **8**, 197–202 (1976).

Variables:
T/K = 297.96–313.00
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
297.96	74.41	1.156	1.261
298.00	74.31	1.154	1.260
298.01	74.48	1.158	1.263
298.11	74.93	1.165	1.271
313.00	65.79	1.006	1.153

The compiler calculated the Bunsen coefficients, assuming ideal gas and Henry's law behavior.
Smoothed data for use between 297.96 K and 313.00 K: $\ln x_1 = -7.5045 + 7.7647/(T/100\ \mathrm{K})$.

T/K	$10^4 x_1$
298.15	74.45
308.15	68.42

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by the difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) *trans*-1,2-Dimethylcyclohexane. Chemical Samples Co. Fractionally distilled and stored in the dark. Refractive index (NaD, 298.15 K) 1.4248.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) *trans*-1,3-Dimethylcyclohexane, 41 mol %; C_8H_{16} ; [2207-03-6]
(3) *cis*-1,3-Dimethylcyclohexane, 59 mol %; C_8H_{16} ; [638-04-0]

Original Measurements:

E. B. Geller, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **8**, 197–202 (1976).

Variables:

T/K = 298.07, 312.97
p_1 /kPa = 101.325

Prepared By:

H. L. Clever

Experimental Data

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
298.07	76.39	1.183	1.291
312.97	63.40	0.888	1.017

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior. The solubility values were adjusted to a sulfur hexafluoride partial pressure of 101.325 kPa by Henry's law.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:

(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) *trans*-1,3-Dimethylcyclohexane.
(3) *cis*-1,3-Dimethylcyclohexane. Chemical Samples Co. Purchased as binary mixture, used as received. Authors analyzed mixture by refractive index.

Estimated Error:

δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:

[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) *trans*-1,4-Dimethylcyclohexane, 30 mol %; C_8H_{16} ; [2207-04-7]
(3) *cis*-1,4-Dimethylcyclohexane, 70 mol %; C_8H_{16} ; [624-29-3]

Original Measurements:

E. B. Geller, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **8**, 197–202 (1976).

Variables:

T/K = 298.36, 312.96
p_1 /kPa = 101.325

Prepared By:

H. L. Clever

Experimental Data

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
298.36	75.15	1.168	1.276
312.96	64.61	0.988	1.132

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior. The solubility values were adjusted to a sulfur hexafluoride partial pressure of 101.325 kPa by Henry's law.

Auxiliary Information

Method/Apparatus/Procedure:

The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:

(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) *trans*-1,4-Dimethylcyclohexane.
(3) *cis*-1,4-Dimethylcyclohexane. Chemical Samples Co. Purchased as binary mixture, used as received. Authors analyzed mixture by refractive index.

Estimated Error:

δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:

[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) *cis*-Decahydronaphthalene (*cis*-decalin); $C_{10}H_{18}$; [493-01-6] or
trans-Decahydronaphthalene (*trans*-decalin); $C_{10}H_{18}$; [493-02-7]

Original Measurements:

L. E. W. Horsman-van den Dool, and J. W. Warman, Interuniversity Reactor Institute (IRI)-Report 134-81-01

Variables:

T/K = 291.2–299.4
p_1 /kPa = not given.

Prepared By:

H. L. Clever

Experimental Data

Solvent	t/°C	T/K	Ostwald Coefficient (L/cm^3 cm^{-3})	Number Of Runs
cis-Decalin	26.2	299.4	0.52	3
trans-Decalin	18.0	291.2	0.71	3
trans-Decalin	21.3	294.5	0.69	3
trans-Decalin	25.0	298.2	0.68	1

Auxiliary Information

Method/Apparatus/Procedure:

A cylindrical glass container of approximately 15 cm^3 volume is filled with solvent and closed with a half-hole septum. An amount of gaseous solute is added to the container. The closed container is shaken for 30 min. Samples of both the vapor and liquid phases are taken in calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.
The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 20 cm Porapack Q column is used for the separation.

Source and Purity of Material:

(1) Sulfur hexafluoride. Baker Chemical Co. Instrument Grade, 99.9%. Used as received.
(2) *cis*-Decalin and *trans*-Decalin. Merck and Co. Zur Synthese grade.
Impurities in both solvents which give the same retention time as the solute gas are removed before the experiment by absorption or distillation.

Estimated Error:

$\delta L/L = \pm 0.05$

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Cyclooctane; C_8H_{16} ; [292-64-8]

Original Measurements:

R. J. Wilcock, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **9**, 111–115 (1977).

Variables:

T/K = 289.23–313.43
p_1 /kPa = 101.325

Prepared By:

H. L. Clever

Experimental Data

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
289.23	28.40	0.4713	0.4990
298.21	29.50	0.4861	0.5307
313.43	25.92	0.4212	0.4833

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 288.15 K and 313.15 K: $\ln x_1 = -7.1556 + 3.8205/(T/100\ \text{K})$.
The standard error about the regression line is 1.70×10^{-4}.

T/K	$10^4 x_1$
288.15	29.4
298.15	28.1
308.15	27.0

Auxiliary Information

Method/Apparatus/Procedure:

The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:

(1) Sulfur hexafluoride. Air Products and Chemicals, Inc. Minimum mole % purity is 99.8.
(2) Cyclooctane. Chemical Samples Co. 99 mole %, distilled, refractive index (NaD, 298.15 K) 1.4562.

Estimated Error:

δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1 = \pm 0.005$

References:

[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Benzene; C_6H_6 ; [71-43-2]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 280.82–305.66
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

t/°C	T/K	$10^3 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
7.67	280.82	2.860	0.734	0.755
16.12	289.27	2.746	0.698	0.739
24.88	298.03	2.641	0.664	0.724
32.51	305.66	2.553	0.636	0.712

The compiler calculated the Bunsen and Ostwald coefficient values, assuming an ideal gas and Henry's law behavior.
Smoothed data, for use between 280.82 K and 305.66 K: $\ln x_1 = -7.2503 + 3.9131/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.52×10^{-6}.

T/K	$10^3 x_1$
283.15	2.828
288.15	2.761
298.15	2.638
303.15	2.581

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2 , evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilbration is attained within 24 h.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be minimum purity of 99 mol %, further purified by sublimation.
(2) Benzene. Brothers Chemical Co. Analytical reagent grade. Shaken successively with concentration H_2SO_4 , 5% NaOH solution and water (twice). Dried over Oronite and distilled.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.002$ (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1,1′-Bicyclohexyl; $C_{12}H_{22}$; [92-51-3] or Benzene; C_6H_6 ; [71-43-2]

Original Measurements:
L. E. W. Horsman-van den Dool and J. W. Warman, Interuniversity Reactor Institute (IRI)-Report 134-81-01.

Variables:
T/K = 295.0, 296.2
P_1 /kPa = not given.

Prepared By:
H. L. Clever

Experimental Data

Solvent	t/°C	T/K	Ostwald Coefficient (L/cm^3 cm^{-3})	Number Of Runs
1,1′-Bicyclohexyl	23.0	296.2	0.51	2
Benzene	21.8	295.0	0.71	3

Auxiliary Information

Method/Apparatus/Procedure:
A cylindrical glass container of approximately 15 cm^3 volume is filled with solvent and closed with a half-hole septum. An amount of gaseous solute is added to the container. The closed container is shaken for 30 min. Samples of both the vapor and liquid phases are taken in calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.
The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 20 cm Porapack Q column is used for the separation.

Source and Purity of Material:
(1) Sulfur hexafluoride. Baker Chemical Co. Instrument Grade, 99.9%. Used as received.
(2) 1.1′-Bicyclhexyl. Fluka. Purum grade.
Benzene. Merck and Co. Uvasol Fluoreszenzspektroskopie grade.
Impurities in both solvents which give the same retention time as the solute gas are removed before the experiment by absorption or distillation.

Estimated Error:
$\delta L / L = \pm 0.05$

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2251-62-4]
(2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18} ; [540-84-1]
(3) Benzene; C_6H_6 ; [71-43-2]

Original Measurements:
D. A. Armitage, R. G. Linford, and D. G. T. Thornhill, J. Chem. Thermodyn. **15**, 225–230 (1983).

Variables:
T/K = 302.75
p_1 /MPa = 0.101325
x_3 = 0 – 1.0

Prepared By:
H. L. Clever

Experimental Data

The solubility of SF_6 at 302.75 K in the mixed solvents follows:

Mole Fraction Benzene/x_3	Mole Fraction $SF_6/10^4 x_1$
1.000	25[a]
0.800	49.3
0.700	61.5
0.599	72.1
0.500	85.1
0.399	96.3
0.300	111.6
0.196	125.5
0.100	133.6
0.0	138.0

[a]Value not given in the paper and was therefore estimated by compiler from author's figure.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Dymond and Hildebrand.[1] It consists of a solvent measuring buret and a manometer constructed of precision bore tubing, a mixing vessel of known volume (370 ± 1) cm^3, and a second manometer. A liquid nitrogen-cooled sorption vacuum pump is used. The whole apparatus is in an air bath. Dry gas is first introduced into the mixing vessel and its amount determined by a pressure measurement. The first degassed solvent is passed into the solvent buret and a measured volume transferred to the mixing vessel. The first solvent is pumped from the buret and the second degassed solvent is added to the solvent buret. Successive measured aliquots are transferred to the mixing vessel until the desired mole fraction range is covered, equilibration taking place after each addition.

Source and Purity of Material:
(1) Sulfur hexafluoride. Cambrian Chemicals. Stated to be 99.9 mole %.
(2) Isooctane. British Drug Houses. "Spectro-quality." Stated to be 99 mole %.
(3) Benzene. British Drug Houses. Stated to be 99.8 mole %.

Estimated Error:
δT/K = ± 0.05
$\delta x_1 / x_1$ = ± 0.013 (authors).

References:
[1]J. H. Dymond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Methylbenzene (toluene); C_7H_8 ; [108-88-3]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 281.06 – 307.57
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

t/°C	T/K	$10^3 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
7.91	281.05	3.810	0.817	0.841
14.49	287.64	3.671	0.782	0.841
24.90	298.05	3.403	0.782	0.781
34.42	307.57	3.193	0.665	0.749

The compiler calculated the Bunsen and Ostwald coefficient values, assuming an ideal gas and Henry's law behavior.
Smoothed data, for use between 281.06 K and 307.57 K: $\ln x_1 = -7.6434 + 5.8401/(T/100\ \mathrm{K})$.
The standard error about the regression line is 2.01×10^{-5}.

T/K	$10^3 x_1$
283.15	3.769
288.15	3.637
298.15	3.398
308.15	3.189

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2 , evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilbration is attained within 24 h.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be minimum purity of 99 mol %, further purified by sublimation.
(2) Methylbenzene. Brothers Chemical Co. Analytical reagent grade. Shaken successively with concentration H_2SO_4 , Water, 5% NaOH solution, water and mercury. Dried over P_2O_5 and distilled.

Estimated Error:
$\delta x_1 / x_1$ = ± 0.002 (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1,2-Dimethylbenzene (xylene); C_8H_{10} ; [95-47-6]

Original Measurements:
J. E. Byrne, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **7**, 515–522 (1975).

Variables:
T/K = 283.09–313.43
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Data

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
283.09	35.04	0.6595	0.6835
283.20	34.81	0.6551	0.6792
298.16	31.18	0.5783	0.6313
313.07	28.49	0.5210	0.5971
313.07	28.69	0.5245	0.6012
313.15	28.61	0.5231	0.5997

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data, for use between 283.09 K and 313.15 K: $\ln x_1 = -7.7442 + 5.9049/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.55×10^{-5}.

T/K	$10^4 x_1$
283.15	34.87
293.15	32.47
298.15	31.39
303.15	30.39
313.15	28.55

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Either Air Products and Chemicals, Inc. or Matheson Co. Inc. 99 mole % or better.
(2) 1,2-Dimethylbenzene. Phillips Petroleum Co. Pure grade.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1,3-Dimethylbenzene or *m*-xylene; C_8H_{10} ; [108-38-3]

Original Measurements:
J. E. Byrne, R. Battino and E. Wilhelm, J. Chem. Thermodyn. **7**, 515–522 (1975).

Variables:
T/K = 282.87–313.20
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3}atm^{-1}]	Ostwald Coefficient (L/cm^{3}cm^{-3})
282.87	40.62	0.7516	0.7783
283.00	40.48	0.7489	0.7759
298.20	36.28	0.6614	0.7212
298.20	36.25	0.6601	0.7206
313.18	32.92	0.5904	0.6770
313.19	33.39	0.5989	0.6867
313.20	33.04	0.5926	0.6795

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data, for use between 282.87 and 313.20 K: $\ln x_1 = -7.6041 + 5.9270/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.55×10^{-5}.

T/K	$10^4 x_1$
283.15	40.43
283.15	37.64
298.15	36.39
303.15	35.91
313.15	33.08

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Either Air Products and Chemicals, Inc. or Matheson Co. Inc. 99 mole % or better.
(2) 1,3-Dimethylbenzene. Phillips Petroleum Co. Pure grade.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1,4-Dimethylbenzene or *p*-xylene; C_8H_{10} ; [106-42-3]

Original Measurements:
J. E. Byrne, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **7**, 515–522 (1975).

Variables:
T/K = 288.10–313.15
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
288.10	40.05	0.7348	0.7750
288.15	40.20	0.7374	0.7779
298.18	36.49	0.7374	0.7230
298.21	37.14	0.6741	0.7359
313.14	34.24	0.6120	0.7016
313.15	33.76	0.6033	0.6916
313.15	33.31	0.5953	0.6825

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data, for use between 288.10 K and 313.15 K: $\ln x_1 = -7.6041 + 5.9270/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.55×10^{-5}.

T/K	$10^4 x_1$
293.15	38.49
298.15	38.49
303.15	35.92
313.15	33.68

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Either Air Products and Chemicals, Inc. or Matheson Co. Inc. 99 mole % or better.
(2) 1,4-Dimethylbenzene. Phillips Petroleum Co. Pure grade.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1-Alkanols (C_1 to C_{11}),
Methanol; CH_3OH; [67-56-1]
Ethanol; C_2H_5OH; [64-17-5]
1-Propanol; C_3H_7OH; [71-23-8]
1-Butanol; C_4H_9OH; [71-36-3]
1-Pentanol; $C_5H_{11}OH$; [71-41-0]
1-Hexanol; $C_6H_{13}OH$; [111-27-3]
1-Heptanol; $C_7H_{15}OH$; [111-70-6]
1-Octanol; $C_8H_{17}OH$; [111-87-5]
1-Nonanol; $C_9H_{19}OH$; [143-08-8]
1-Decanol; $C_{10}H_{21}OH$; [112-30-1]
1-Undecanol; $C_{11}H_{23}OH$; [112-42-5]

Original Measurements:
S. Bo, R. Battino, and E. Wilhelm, J. Chem. Eng. Data **38**, 611–616 (1993).

Variables:
T/K = 298.15
p_1 /MPa = 0.101325

Prepared By:
H. L. Clever

Experimental Values

Ostwald coefficient and Henry fugacity of sulfur hexafluoride at 298.15 K and a *total* pressure of 101 325 Pa. The sulfur hexafluoride mole fraction solubility at 298.15 K and a *partial* pressure of 101 325 Pa

Alkanol	Ostwald Coefficient [$L_{1,2}(T,p)$]	Henry Fugacity ($10^{-6} H_{1,2} T, p_{s,2}$)/Pa	$10^4 x_1$
Methanol	0.6178	95.86	10.44
Ethanol	0.7505	54.78	18.24
1-Propanol	0.7377	43.53	22.94
1-Butanol	0.6775	38.75	25.76
1-Pentanol	0.6180	35.97	27.75
1-Hexanol	0.5624	34.29	29.11
1-Heptanol	0.5366	31.77	31.42
1-Octanol	0.5031	30.33	32.91
1-Nonanol	0.4812	28.73	34.75
1-Decanol	0.4527	27.91	35.77
1-Undecanol	0.4351	26.77	37.30

Alkanol properties listed and used by the authors are given below (see the paper for references).

1 (alkanol)	2	3	4	5	6	7	8	9	10
Methanol	16941	0.7866	1.195	1348	285	0.564	512.3	8.092	117.8
Ethanol	7876	0.7851	1.093	1153	281	0.643	514.1	6.140	166.9
1-Propanol	2786	0.7996	0.995	1006	281	0.620	536.7	5.168	218.5
1-Butanol	858	0.8058	0.932	942	281	0.591	562.4	4.418	274.5
1-Pentanol	259	0.8111	0.893	884	301	0.579	588.0	3.868	326.5
1-Hexanol	77	0.8154	0.870	836	310	0.575	611.0	3.413	393.0
1-Heptanol	77	0.8194	0.861	800	321	0.580	632.5	3.058	435.2
1-Octanol	6	0.8218	0.854	777	328	0.594	652.6	2.777	506.7
1-Nonanol	2	0.8245	0.826	752	327	0.610	670.5	2.546	572.4
1-Decanol	>1	0.8266	0.812	733	330	0.629	687.1	2.330	648.7
1-Undecanol	>1	0.8292	0.813	723	335	0.656	703.3	2.147	718.0

The properties given in columns 2–10 of the above table are defined below according to column number.

1	Alkane	2	Vapor pressure, $p_{s,2}$ /Pa
3	Density, $10^{-3}\rho_2{}^L$/(kg m^{-3})	4	Isobaric expansivity, $10^3 \alpha_{p,2}{}^L$/K^{-1}
5	Isothermal compressibility, $10^{12}\beta_{T,2}{}^L$/Pa^{-1}	6	Internal pressure, $10^{-6}\Pi_2{}^L$/Pa
7	Acentric factor, ω_2	8	Critical temperature, $T_{c,2}$ /K
9	Critical pressure, $10^{-6} p_{c,2}$ /Pa	10	Critical molar volume, $10^6 V_{c,2}$ /(m^3 mol^{-1})

Auxiliary Information

Method/Apparatus/Procedure:

The solubility were measured with a Ben-Naim/Baer type apparatus as modified by the Tominaga *et al.*[1] The apparatus has four equilibration cells of ~26, 65, 380, and 1650 cm^3 volume for different ranges of Ostwald coefficients. The equilibration vessels and the gas burettes were calibrated with doubly distilled water, and the respective volumes are known to ± 0.01 cm^3. The total pressure was determined with a pressure transducer. The entire apparatus is in a large air thermostat controlled to better than ± 0.01 K. Temperatures were measured by a calibrated platinum resistance cell based on IPTS-68. Prior to measurement the solvents were degassed by the method of Battino *et al.*[2] and transferred under their own vapor pressure into the solubility apparatus.

Source and Purity of Materials:

(1) Sulfur hexafluoride. Either Matheson or Airco. Minimum mole % purity stated to be 99.8.
(2) 1-Alkanols.
Methanol, Fisher Certified grade.
Ethanol, Pharmco (USP 200 Proof).
1-Propanol, Fisher Certified grade. (99.8%).
1-Butanol, Fisher Certified grade.
1-Pentanol, Fisher Certified grade (99.3%).
1-Hexanol, Fisher Certified grade (99.6%).
1-Heptanol, Fisher Certified grade (99.6%).
1-Octanol, Fisher Certified grade (99.3%).
1-Nonanol, Fluka.
1-Decanol, Fluka.
1-Undecanol, Fluka.
All alkanols were distilled at least once through a 1.2 m vacuum jacketed packed column at a reflux ratio of 15 or better. The middle 80% of the distillate was used for the solubility measurements. The refractive index of each purified alkanol agreed well with reliable literature values. The purities in the table above were determined by gas chromatography.

Estimated Error:

$\delta T/K = \pm 0.1$
$\delta x_1/x_1 = \pm 0.002$ (authors).

References:

[1]T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[2]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6; [2551-64-4]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:

J. Pardo, M. C. Lopez, J. Santafe, F. M. Royo and J. S. Urieta, Fluid Phase Eq. **109**, 29–37 (1995).

Variables:

$T/K = 263.15–303.15$
$p_1/kPa = 101.33$

Prepared By:

H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
263.15	37.26	0.9414	0.9069
273.15	32.81	0.8210	0.8210
283.15	28.84	0.7147	0.7409
293.15	25.75	0.6320	0.6783
298.15	24.54	0.5994	0.6543
303.15	23.43	0.5695	0.6321

The compiler calculated the Bunsen and Ostwald coefficients from the authors mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation:

$$\ln x_1 = -9.1470 + 935.222/(T/K) \quad (\sigma = 0.0057).$$

From this equation they obtained $\Delta H°_1$ /kJ $mol^{-1} = -7.78$ and $\Delta S°_1$ /J K^{-1} $mol^{-1} = -76$ for the transfer of 1 mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas.

Source and Purity of Material:

(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) 1-Butanol. Aldrich Chemical Co. Purity checked by GLC to be 99.8%.

Estimated Error:

$\delta T/K = \pm 0.05$ cell; $= \pm 0.2$ burets.
$\delta x_1/x_1 = \pm 0.007$ (authors).

References:

[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]

Original Measurements:
J. Pardo, M. C. Lopez, J. A. Mayoral, F. M. Royo, and J. S. Urieta, Fluid Phase Eq. **134**, 133–140 (1997).

Variables:
T/K = 263.15–303.15
p_1 /kPa = 101.33

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient (α/cm^3 (STP) cm^{-3} atm^{-1})	Ostwald Coefficient (L/cm^3 cm^{-3})
263.15	48.75	1.234	1.188
273.15	41.97	1.050	1.050
283.15	37.17	0.920	0.954
293.15	33.19	0.813	0.872
298.15	31.37	0.764	0.834
303.15	29.83	0.722	0.802

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation: $\ln x_1 = -9.0279 + 972.984/(T/\mathrm{K})$ ($\sigma = 0.0063$).

From this equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −8.09 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −73 for the transfer of one mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the table for experimental values in the paper.

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) 2-Butanol. Aldrich Chemical Co. Purity checked by GLC to be 99%.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

Original Measurements:
J. Pardo, M. C. Lopez, J. Santafe, F. M. Royo, and J. S. Urieta, Fluid Phase Eq. **119**, 165–173 (1996).

Variables:
T/K = 263.15–303.15
p_1 /kPa = 101.33

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
263.15	50.70	1.2703	0.7336
273.15	43.72	1.0846	1.0846
283.15	38.65	0.9494	0.9841
293.15	34.04	0.8279	0.8885
298.15	32.17	0.7786	0.8498
303.15	30.46	0.7336	0.8141

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation: $\ln x_1 = -9.1425 + 1014.652/(T/\mathrm{K})$ ($\sigma = 0.0039$).

From this equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −8.84 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −76 for the transfer of one mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the Table in the paper.

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) 2-Methy-propanol. Aldrich Chemical Co. Purity checked by GLC to be 99.5%.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Methanol; CH_4O; [67-56-1]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
N. Brückl and J. I. Kim, Z. Phys. Chem. (Wiesbaden) **133**, 133–150 (1981).

Variables:
T/K = 298.2
p_1 /MPa = 0.1013

Prepared By:
C. L. Young

Experimental Values

Solvent (T/K)	Henry's Constant ln[K_H /atm]	$10^3 x_1$
Methanol (298.2)	6.74	1.18
Ethanol (298.2)	6.20	2.03

The compiler calculated the mole fraction solubility at a partial pressure of 1 atm (0.1013 MPa) assuming $x_1 = 1/K_H$.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilies were determined by a volumetric method described as "the Ostwald method." No other details given.

Source and Purity of Material:
(1) Sulfur hexafluoride. Linde Co. Purity stated to be 99.8 volume %.
(2) Methano and Ethanol. Uvasol or analytical grade.

Estimated Error:
δT/K = ±0.1
δK_H = ±1.25%

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]

Original Measurements:
J. Pardo, A. M. Mainar, M. C. Lopez, F. M. Royo, and J. S. Urieta, Fluid Phase Eq. **155**, 127–137 (1999).

Variables:
T/K = 303.15
p_1 /kPa = 101.33

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
303.15	44.52	1.06	1.18

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. The solubility of the gas has been derived from the experimental data by applying a reduction method[3] based on that proposed by Wilhelm.[4]
Note that the temperature range considered for the other butyl alcohol isomers could not be used for the t-butyl alcohol because of its freezing point of 298.77 K.

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) 2-Methyl-2-propanol or t-butyl alcohol. Aldrich Chemical Co. Purity stated to be 99.5%. Checked by GLC.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).
[3]F. Gibanel, M. C. Lopez, F. Royo, V. Rodriguez, and J. S. Urieta, J. Solution Chem. **23**, 1061 (1994).
[4]E. Wilhelm, CRC Critical Reviews in Analytical Chemistry **16**(1–2), 129 (1985).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

Original Measurements:
R. J. Wilcock, R. Battino, W. F. Danforth, and E. Wilhelm, J. Chem. Thermodyn. **10**, 817–822 (1978).

Variables:
T/K = 282.61–313.48
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
282.61	37.81	0.5367	0.5553
298.15	32.86	0.4613	0.5035
313.48	28.69	0.3979	0.4567

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data, for use between 283.15 K and 313.15 K: $\ln x_1 = -8.3767 + 7.9151/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.55×10^{-4}.

T/K	$10^4 x_1$
283.15	37.68
293.15	34.25
298.15	32.73
303.15	31.33
303.15	28.82

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) 1-Octanol. Eastman Organic Chemicals. Distilled, density at 298.15 K, ρ/g cm^{-3} = 0.8247.

Estimated Error:
δT/K = ±0.02
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1-Decanol; $C_{10}H_{22}O$; [112-30-1]

Original Measurements:
R. J. Wilcock, R. Battino, W. F. Danforth, and E. Wilhelm, J. Chem. Thermodyn. **10**, 817–822 (1978).

Variables:
T/K = 283.20–313.45
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient L/cm^3 cm^{-3}
283.20	38.98	0.4572	0.4740
298.28	35.62	0.4135	0.4515
313.45	30.42	0.3490	0.4005

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data: for use between 283.15 K and 313.15 K: $\ln x_1 = -8.0908 + 7.2390/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.14×10^{-4}.

T/K	$10^4 x_1$
283.15	39.5
293.15	36.2
298.15	34.7
303.15	33.4
303.15	30.9

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) 1-Decanol. Eastman Organic Chemicals. Distilled, density at 298.15 K, ρ/g cm^{-3} = 0.8206.

Estimated Error:
δT/K = ±0.02
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [75-89-8]

Original Measurements:

A. M. Mainar, J. Pardo, F. M. Royo, M. C. Lopez, and J. S. Urieta, J. Solution Chem. **25**, 589–595 (1996).
M. A. Sanchez, A. M. Mainar, J. I. Pardo, M. C. Lopez, and J. S. Urieta, Can. J. Chem. **79**, 1460–1465 (2001).

Variables:

T/K = 268.15, 283.15 and 298.15
p_1 /kPa = 101.32

Prepared By:

H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
268.15	89.88	2.91	2.86
283.15	68.45	2.17	2.25
298.15	55.48	1.73	1.89

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction and density values using the solvent density in the paper and assuming ideal gas behavior. The 268.15 K and 283.15 K values are from the 2001 paper and the 298.15 K value is from the 1996 paper.

The authors fitted the data to the equation: $\ln x_1 = -9.521 + 1287.91/(T/\mathrm{K})$ with $r^2 = 0.9980$.

Calculated from the equation: $\Delta H°$ /kJ mol^{-1} = 10.71 and $\Delta S°$ /J K^{-1} mol^{-1} = −73.

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a five buret system, a pressure transducer system, and a solution vessel of 85 cm^3 for the CF_4 and of 27 cm^3 for the SF_6 . The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. To reduce the data from the working pressure to 101.33 kPa the following simplifications are assumed:
1. the liquid activity coefficients are assumed to be unity,
2. the fugacity coefficients can be obtained from a virial equation truncated after the second term, and
3. for the partial molar volumes in the Poynting correction the average values reported[3] were used for gases and the value calculated from the liquid density of the solvent was used for the solvent.

Source and Purity of Material:

(1) Sulfur hexafluoride. Air Liquide España stated to be 99.5%.
(2) 2,2,2-Trifluoroethanol. Janssen Chimica. Purity stated to be 99%. Purity checked by GLC.

Estimated Error:

δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.01 (authors).

References:

[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).
[3]R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids* (McGraw–Hill, New York, 1986).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) 1,1,1,3,3,3-Hexafluoropropan-2-ol; $C_3H_2F_6O$; [920-66-1]

Original Measurements:

A. M. Mainar, J. Pardo, J. I. Garcia, F. M. Royo, and J. S. Urieta, J. Chem. Soc., Faraday Trans. **94**, 3595–3599 (1998).
M. A. Sanchez, A. M. Mainar, J. A. Pardo, M. C. Lopez, and J. S. Urieta, Can. J. Chem. **79**, 1460–1465 (2001).

Variables:

T/K = 268.15, 283.15, and 298.15
p_1 /kPa = 101.32

Prepared By:

H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
268.15	230.9	5.30	5.20
283.15	186.4	4.13	4.28
298.15	143.5	4.13	3.40

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction and density values using the solvent density in the paper and assuming ideal gas behavior. The 268.15 K and 283.15 K values are from the 2001 paper and the 298.15 K value is from the 1996 paper.

The authors fitted the data to the equation: $\ln x_1 = -9.421 + 1542.68/(T/\mathrm{K})$ with $r^2 = 0.9989$.

From the equation, $\Delta H°$/kJ mol^{-1} = −12.82 and $\Delta S°$/J K^{-1} mol^{-1} = −78.

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a five buret system, a pressure transducer system, and a solution vessel of 85 cm^3 for the CF_4 and of 27 cm^3 for the SF_6 . The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. To reduce the data from the working pressure to 101.33 kPa the following simplifications are assumed: (1) The liquid activity coefficients are assumed to be unity, (2) the fugacity coefficients can be obtained from a virial equation truncated after the second term, and (3) for the partial molar volumes in the Poynting correction the average values reported[3] were used for gases and the value calculated from the liquid density of the solvent was used for the solvent.

Source and Purity of Material:

(1) Sulfur hexafluoride. Air Liquide España. Stated to be 99.5%.
(2) Hexafluoropropan-2-ol. Fluorchem Ltd. Purity stated to be >99%. Checked by GLC. At 298.15 K: Density 1604.23 kg m^{-3}. Vap P 21.17 kPa from literature.

Estimated Error:

δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.01 (authors).

References:

[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).
[3]R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids* (McGraw–Hill, New York, 1986).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 2-Propanone or acetone; C_3H_6O; [67-64-1] and
4-Methyl-1,3-dioxolan-2-one (propylene carbonate); $C_4H_6O_3$; [108-32-7]

Original Measurements:
N. Brückl and J. I. Kim, Z. Phys. Chem. (Wiesbaden) **133**, 133–150 (1981).

Variables:
T/K = 298.2
p_t /MPa = 0.1013

Prepared By:
C. L. Young

Experimental Values

Solvent	T/K	Henry's Constant [ln(K_H /atm)]	$10^3 x_1$
2-Propanone	298.2	298.2	3.41
Propylene carbonate	298.2	7.32	0.662

The compiler calculated the mole fraction solubility at a partial pressure of 1 atm (0.1013 MPa) assuming $x_1 = 1/K_H$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by a volumetric method described as "the Ostwald method." No other details given.

Source and Purity of Material:
(1) Sulfur hexafluoride. Linde Co. Purity stated to be 99.8 vol %.
(2) 2-Propanone and 4-Methyl-1,3-dioxolane-2-one: Uvasol or analytical grade.

Estimated Error:
δT/K = ±0.1
δK_H = ±1.25%

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Cyclopentanone; C_5H_8O; [120-92-3]

Original Measurements:
M. A. Gallardo, M. C. Lopez, J. S. Urieta, and C. Gutierrez-Losa, Fluid Phase Equil. **50**, 223–233 (1989).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
C. L. Young

Experimental Values

T/K	Henrys Coefficient [10^4 atm/$H_{2,1}$ corrected (uncorrected)]	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	18.29 (17.90)	0.4631	0.4631
283.15	17.28 (16.90)	0.4329	0.4487
293.15	16.44 (16.07)	0.4074	0.4372
298.15	15.94 (15.58)	0.3930	0.4289
303.15	15.52 (15.17)	0.3806	0.4224

The compiler calculated the Bunsen and Ostwald coefficients from the authors uncorrected Henry's coefficients. See source for definition of corrected Henry's coefficient. Density data were taken from the literature.[2] Ideal gas behavior was assumed. The uncorrected column above is equal to the mole fraction solubility at 101.325 kPa.
The authors fitted their data to the equation: $\ln H_{2,1}/101.32\ \text{kPa} = 7.9538 + 451.06/(T/\text{K})$.
From the equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −3.75 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −66 at 298.15 K and a partial pressure of 101.32 kPa.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors[1] have described their apparatus in an earlier paper. The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent saturated gas. It appears that the mole fraction solubility at 1 atm was estimated from the raw data by assuming Henry's law is obeyed and that the partial pressure of the solvent is given by Raoult's law.

Source and Purity of Material:
(1) Sulfur hexafluoride: Sociedad Español del Oxigeno sample. Purity stated to be 99.5 mol %.
(2) Cyclopentanone. Fluka. Purity stated to be 98.5 mole %.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.02 (authors).

References:
[1] J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2] J. Timmermans, *Physico-Chemical Constants of Organic Compounds* (Elsevier, Amsterdam).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]

Original Measurements:
M. A. Gallardo, J. M. Melendo, J. S. Urieta, and C. Gutierrez Losa, Can. J. Chem. **65**, 2198–2202 (1987).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient L/cm^3 cm^{-3}
273.15	20.5	0.453	0.453
283.15	19.3	0.423	0.438
293.15	18.2	0.395	0.424
298.15	17.7	0.382	0.417
303.15	17.2	0.369	0.410

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation: $\ln x_1 = 3.072 - 1.6511 \ln(T/\mathrm{K})$ $(10^4\sigma = 0.014)$.

From the equation they obtained ΔH°_1 /kJ mol^{-1} = −4.09 and ΔS°_1 /J K^{-1} mol^{-1} = −66 for the transfer of 1 mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the table in the paper.

Source and Purity of Material:
(1) Sulfurhexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5% pure.
(2) Cyclohexanone. Carlo Erba. Refractive index n_D (293.15 K) = 1.45071. Purity checked by GLC found to be at least 99%.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.02 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) 2-Methylcyclohexanone; $C_7H_{12}O$; [583-60-8]

Original Measurements:
M. A. Gallardo, M. C. Lopez, J. S. Urieta, and C. Gutierrez Losa, Can. J. Chem. **67**, 809 811 (1989).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	31.9	0.603	0.603
283.15	29.2	0.546	0.566
293.15	27.1	0.502	0.539
298.15	26.3	0.485	0.530
303.15	25.2	0.463	0.513

The compiler calculated the Bunsen and Ostwald coefficients from the authors mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation: $\ln x_1 = 8.0784 + 635.96/(T/\mathrm{K})$ $(\sigma = 0.0029)$.

From the equation they obtained ΔH°_1 /kJ mol^{-1} = −5.29 and ΔS°_1 /J K^{-1} mol^{-1} = −67 for the transfer of 1 mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer.[1] The authors have described their apparatus in an earlier paper.[2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the Table in the paper.
The vapor pressure of 2-methylcyclohexanone was determined and fitted to the equation:
$\ln(p_2/\mathrm{kPa}) = -5552.37/(T/\mathrm{K}) + 18.046$

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5% pure.
(2) 2-Methylcyclohexanone. Merck and Co. Refractive index n_D (293.15 K) = 1.44766. Purity checked by GLC to be at least 98.1% pure. Cyclohexanone 0.6% was found as an impurity.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735–38 (1963).
[2]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) Cycloheptanone; $C_7H_{12}O$; [502-42-1]

Original Measurements:
M. A. Gallardo, M. C. Lopez, J. S. Urieta, and C. Gutierrez-Losa, Fluid Phase Equil. **58**, 159–172 (1990).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	19.76	3.838	3.838
283.15	18.57	3.575	3.706
293.15	17.60	3.358	3.604
298.15	17.16	3.259	3.557
303.15	17.16	3.184	3.534

The compiler calculated the Bunsen and Ostwald coefficients from the authors mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation: $\ln x_1 = -7.8565 + 444.47/(T/\mathrm{K})$.

From the equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −3.70 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −65 for the transfer of 1 mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier paper.[1] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent saturated gas. It appears that the mole fraction solubility at 1 atm was estimated from the raw data by assuming Henrys law is obeyed and that the partial pressure of the solvent is given by Raoults law.
Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the Table in the paper.

Source and Purity of Material:
(1) Sulfurhexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5% pure.
(2) Cycloheptanone. Merck and Co. sample. Purity stated to be 99.2 mole %.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) 2,6-Dimethylcyclohexanone; $C_8H_{14}O$; [2816-57-1]

Original Measurements:
M. A. Gallardo, M. C. Lopez, J. S. Urieta, and C. Gutierrez Losa, Can. J. Chem. **68**, 435–439 (1990).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.33

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	44.0	0.792	0.792
283.15	39.8	0.653	0.677
293.15	36.4	0.592	0.635
298.15	35.0	0.566	0.618
303.15	33.8	0.545	0.604

The compiler calculated the Bunsen and Ostwald coefficients from the authors mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation: $\ln x_1 = -8.1076 + 731.60/(T/\mathrm{K})$ ($\sigma = 0.0033$).

From the equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −6.08 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −67 for the transfer of one mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer.[1] The authors have described their apparatus in an earlier paper.[2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values are from the Table in the paper.
The vapor pressure and density of 2,6-dimethyl-cyclohexanone were determined and fitted to the equations:
$\ln(p_2/\mathrm{kPa}) = -3870.53/(T/\mathrm{K}) + 12.861$
and ρ/g cm^{-3} = 0.9290 − 0.0008313(t/°C).

Source and Purity of Material:
(1) Sulfur hexafluoride.
Sociedad Espanola del Oxigeno.
Stated to be 99.5%.
(2) 2,6-Dimethylcyclohexanone.
Fluka.
Refractive index n_D (293.15 K) = 1.44686.
Purity checked by GLC to be at least 98.2%.
A mixture of E and Z (*cis and trans*) isomers.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735–2738 (1963).
[2]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

Original Measurements:
M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. Phys. Biol. **80**, 621–625 (1983).

Variables:
T/K = 285.15–303.15
p_1 /kPa = 101

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^3 atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
285.15	14.7_9	0.3928	0.4101
289.15	14.7_9	0.3861	0.4087
293.15	14.4_7	0.3810	0.4089
298.15	14.2_4	0.3730	0.4071
303.15	14.0_6	0.3662	0.4064

The compiler calculated the Bunsen and the Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $-\ln x_1 = 0.844 \ln(T/\mathrm{K}) + 1.744$,
from which they obtained: $\Delta H°_1$ /kJ mol^{-1} = −2.09 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −62 for the transfer of 1 mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer.[1] It was described in detail in an earlier paper of the authors.[2]
The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent saturated gas.
Literature 1,4-dioxane vapor pressures were fitted to the equation: $\ln(p_2/\mathrm{kPa}) = -4591.3/(T/\mathrm{K}) + 16.98$.

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) 1,4-Dioxane. Merck and Co. Purity checked by GLC to be >99%.

Estimated Error:
δT/K = ±0.1
δp/kPa = ±1
$\delta x_1/x_1$ = ±0.01

References:
[1]A. Ben Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencieas Zaragoza **34**, 115–122 (1973).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Methoxybenzene or anisole; C_7H_8 ; [100-66-3]

Original Measurements:
F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **78**, 171–174 (1981).

Variables:
T/K = 283.15–303.15
p_1 /kPa = 101.3

Prepared By:
C. L. Young

Experimental Values

T/K	$10^4 x_1$
283.15	16.61_1
288.15	16.29_6
293.15	16.01_7
298.15	15.70_0
303.15	15.55_5

The authors smoothing equation is: $\ln x_1 = 0.989 \ln(T/\mathrm{K}) + 0.814$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus was similar to that used by Ben-Naim and Baer,[1] consisting essentially of a gas buret, mercury manometer and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It appears that the mole fraction at a partial pressure of 1 atm was estimated from the raw experimental data by assuming that Henry's law is obeyed and that the partial pressure of the solvent in the gas phase is given by Raoult's law.

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Purity stated to be 99.6 mole %.
(2) Methoxybenzene. Fluka. Purity equal to or better than 99 mole %. Checked by GC.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.04 (estimated by compiler).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Tetrahydrofuran; C_4H_8O; [109-99-9]

Original Measurements:
F. Gibanel, M. C. Lopez, F. M. Royo, J. Santafe, and J. S. Urieta, J. Solution Chem. **22**, 211–217 (1993).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^3 atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	36.50	1.0343	1.0343
283.15	33.98	0.9512	0.9860
293.15	31.62	0.8746	0.9386
298.15	30.71	0.8444	0.9217
303.15	29.52	0.8065	0.8951

The compiler calculated the Bunsen and the Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -7.7359 + 580.322 \ln(T/\mathrm{K})$ ($\sigma = 0.0001041$),
from which they obtained $\Delta H°_1$ /kJ mol^{-1} = 4.83 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −64 for the transfer of 1 mole of SF_6 from the gas phase at 101 kPa to the infinitely dilute solution.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in an earlier paper of the authors.[1,2]
The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel.
Measurements are carried out on the solvent saturated gas.
The vapor pressure of tetrahydrofuran was determined and fitted to the equation: $\ln(p_2/\mathrm{kPa}) = -3914.6/(T/\mathrm{K}) + 23.120$.
The density: ρ/kg m^{-3} = 1199.1 − 1.0640(T/K).

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) Tetrahydrofuran. Fluka. Purity checked by GLC to be 99.5%. R. I. n_D(293.15 K) = 1.40737.

Estimated Error:
δT/K = ±0.05 cell; ±0.2 burets.
δp/kPa = ±1
$\delta x_1/x_1$ = ±0.01

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencieas Zaragoza **34**, 115–122 (1973).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Tetrahydro-2H-pyran; $C_5H_{10}O$; [142-68-7]

Original Measurements:
F. Gibanel, M. C. Lopez, F. M. Royo, V. Rodriguez, and J. S. Urieta, J. Solution Chem. **23**, 1247–1255 (1994).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^3 atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	45.11	1.0644	1.0644
283.15	41.34	0.9644	0.9997
293.15	38.01	0.8766	0.9408
298.15	36.59	0.8390	0.9158
303.15	35.57	0.8109	0.9000

The compiler calculated the Bunsen and the Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -7.8419 + 666.293 \ln(T/\mathrm{K})$ ($10^4\sigma^2 = 0.5$)
from which they obtained: $\Delta H°_1$ /kJ mol^{-1} = −5.54 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −65 for the transfer of 1 mole of SF_6 from the gas phase at 101.3 kPa to the infinitely dilute solution.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in an earlier paper of the authors.[1,2]
The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel.
Measurements are carried out on the solvent saturated gas.
The vapor pressure of tetrahydrofuran was determined and fitted to the equation: $\ln(p_2/\mathrm{kPa}) = -4245.4/(T/\mathrm{K}) + 23.396$.
The density: ρ/kg m^{-3} = 1173.6 − 0.9916(T/K).
Note error in density equation in the paper.

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) Tetrahydro-2H-pyran. Fluka. Purity checked by GLC to be 99%. R. I. n_D(293.15 K) = 1.42086.

Estimated Error:
δT/K = ±0.05 cell; ±0.2 burets.
δp/kPa = ±1
$\delta x_1/x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencieas Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) Tetrahydro-2-methyl-furan; $C_5H_{10}O$; [96-47-9]

Original Measurements:
F. Gibnal, M. C. Lopez, F. M. Royo. J. Pardo, and J. S. Urieta, Fluid Phase Equil. **87**, 285–294 (1993).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	58.70	1.342	1.342
283.15	52.63	1.190	1.234
293.15	48.24	1.079	1.158
298.15	46.05	1.024	1.118
303.15	44.52	0.985	1.093

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -7.9454 + 765.650/(T/\mathrm{K})$ ($\sigma^2 = 0.0055$).
From the equation they obtained ΔH°_1 /kJ mol^{-1} = −6.36 and ΔS°_1 /J K^{-1} mol^{-1} = −66 for the transfer of 1 mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the Table in the paper.
Vapor pressure:
$\ln(p_2/\mathrm{kPa}) = -4103.4/(T/\mathrm{K}) + 23.251$
Density:
ρ/kg m^{-3} = 1118.3 − 0.89765(T/K)

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) Tetrahydro-2-methyl-furan. Fluka. R. I. n_D(293.15 K) = 1.40595. Purity checked by GLC to be > 97%. Vapor pressure and density determined and fitted to equations.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1] J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2] M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) (OC-6-11)-Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-4]
(2) 1,1′-[Methylene*bis*(oxy)]*bis*ethane or formaldehyde diethyl acetal; $C_5H_{12}O_2$; [462-95-3]

Original Measurements:
L. P. Lizano, M. C. Lopez, F. M. Royo, and J. S. Urieta, J. Solution Chem. **19**, 721–728 (1990).

Variables:
T/K = 263.15–303.15
p_1 /kPa = 101.33

Prepared By:
H. L. Clever and C. L. Young

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
263.15	127	2.39	2.30
273.15	108	2.00	2.00
283.15	93.9	1.72	1.78
293.15	81.7	1.47	1.58
298.15	76.8	1.37	1.50
303.15	72.3	1.27	1.41

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -8.6250 + 1119.98/(T/\mathrm{K})$.
From the equation they obtained ΔH°_1 /kJ mol^{-1} = −9.31 and ΔS°_1 /J K^{-1} mol^{-1} = −72 for the transfer of 1 mole of SF_6 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer.[1] The authors have described their apparatus in an earlier paper.[2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values are from the Table in the paper.
The vapor pressure and density of 2,6-dimethyl-cyclohexanone were determined by the authors and fitted to the equations:
$\ln(p_2/\mathrm{kPa}) = -4280.53/(T/\mathrm{K}) + 166.03$ and ρ/g cm^{-3} = 1134.0 − 1.0350(T/K).

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Stated to be 99.5%.
(2) Formaldehyde diethyl acetal. Aldrich Chem. Co. Purity checked by GLC to be at least 99%. Density and vapor pressure determined.

Estimated Error:
$\delta T/K$ = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.02 (authors).

References:
[1] A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735–2738 (1963).
[2] J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Oxepane or hexamethylene oxide; $C_6H_{12}O$; [592-90-5]

Original Measurements:
F. Gibanel, M. C. Lopez, M. H. Gallarado, J. S. Urieta, and C. Gutierrez Losa, Fluid Phase Equilibria **42**, 261–268 (1988).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.3

Prepared By:
C. L. Young

Experimental Values

T/K	Solubility, $10^4 x_1$
273.15	58.3
283.15	52.6
293.15	48.2
298.15	46.0
303.15	44.5

The smoothing equation of the author is: $\ln x_1 = 593.269 \ln(T/\mathrm{K}) - 7.6688$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus was similar to that used by Ben-Naim and Baer,[1] consisting essentially of a gas buret, mercury manometer and solution vessel. The solvent was degassed in the solution vessel.
Measurements were carried out on the saturated gas. It was assumed the mole fraction of solvent in the gas phase was that corresponding to the vapor pressure of the pure solvent. It appears that the mole fraction at a partial pressure of 1 atm was estimated from the raw experimental data by assuming that Henry's law is obeyed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigeno. Purity stated to be 99.5 mole %.
(2) Oxepane. Merck Co. Purity stated to be 99 mole %.

Estimated Error:
δT/K = ±0.02
$\delta x_1 / x_1$ = ±0.02 (estimates by compiler).

References:
[1] A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Tetrachloromethane; CCl_4 ; [56-23-5]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 277.79–304.81
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	$10^3 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
4.64	277.79	8.064	1.92	1.95
14.72	287.87	7.147	1.68	1.77
24.71	307.86	6.579	1.53	1.67
31.66	304.81	6.144	1.42	1.58

The compiler calculated the Bunsen and Ostwald coefficients values assuming an ideal gas and Henry's law behavior.
Smoothed Data, for use between 277.79 K and 304.81 K: $\ln x_1 = -7.8415 + 8.3786/(T/100\ \mathrm{K})$.
The standard error about the regression line is 6.26×10^{-5} and smoothed solubility data are

T/K	$10^3 x_1$
278.15	7.993
288.15	7.199
298.15	6.530

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2 , evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilibration is attained within 24 h.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be minimum purity of 99 mol %, further purified by sublimation.
(2) Tetrachloromethane. Brothers Chemical Co. A. R. Grade. Refluxed over mercury, washed with 5% NaOH and with water, dried over P_2O_5 and distilled.

Estimated Error:
$\delta x_1 / x_1$ = ±0.002 (authors).

References:
[1] Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Tetrachloromethane; CCl_4 ; [56-23-5]

Original Measurements:
T. Tominaga, R. Battino, B. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175–180 (1986).

Variables:
T/K = 298.15
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Ostwald Coefficient $(L/cm^3\ cm)^{-3}$	Henry's Constant $(10^{-6} H/Pa)$
298.15	63.69	1.557	15.91

The compiler calculated the mole fraction value from Henry's Law Constant with no corrections.
Henry's constant, $H/Pa = (p_1/Pa)/x_1$: (101325 Pa = 1 atm).

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Ben-Naim and Baer.[1] It allows no contact between the Hg and CCl_4 . The degassing apparatus is that of Battino *et al.*[2] Degassing. Up to 500 mL of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and a vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm. Solubility Determination. The Ben-Naim and Baer procedure is used. The gas is solvent vapor saturated, dissolution is usually complete within 10–20 m. The mixing volume chambers volumes are 26, 65, 380, and 1650 cm^3 calibrated to $\pm 0.01\ cm^3$. The pressure is maintained constant and the volume changed by a microprocessor controlled stepping motor operating a piston in a precision bore tube.

Source and Purity of Material:
(1) Sulfur hexafluoride. Matheson and Co. Stated to be 99.8 mol % pure.
(2) Tetrachloromethane. Fisher "Certified" grade, 99 mol %. Distilled through a 1.2 m packed column, middle 80% stored protected from light until used.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1 = \pm 0.01$ (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2935 (1963).
[2]R. Battino, M. Banzhof, M. Brogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]

Original Measurements:
M. C. Lopez, M. A. Gallardo, J. S. Urieta, and C. Gutierrez, J. Chem. Eng. Data **32**, 472–474 (1989).

Variables:
T/K = 263.15–303.15
p_1 /bar = 1.013

Prepared By:
C. L. Young

Experimental Values

T/K	$10^4 x_1$
263.15	39.1
273.15	35.7
283.15	32.7
293.15	30.4
303.15	28.4

The authors fitted the data to the equation: $\ln x_1 = -16.3507 + (995.0/(T/K)) + 1.2605 \ln(T/K)$.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility apparatus was similar to that used by Ben-Naim and Baer[1] consisting essentially of a gas buret, mercury manometer, and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It was assumed that the mole fraction of the solvent was that corresponding to the vapor pressure of the pure solvent. It appears that the mole fraction at a partial pressure of 1 atm was estimated from raw experimental data assuming Henry's law is obeyed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigene, S.A. Purity stated to be 99.99 mole %.
(2) Chlorocyclohexane. Merck and Co. Purity 98.5 mole %, main impurity cyclohexane at 0.4 mole %.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1 = \pm 0.015$

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 275.64–305.87
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	$10^3 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
2.49	275.64	4.235	8.54	8.62
14.17	287.32	3.133	6.14	6.46
26.44	299.59	2.707	5.19	5.69
32.72	305.87	2.471	4.68	5.24

The compiler calculated the Bunsen and Ostwald coefficients values assuming an ideal gas and Henry's law behavior.
Smoothed Data for use between 275.64 K and 305.87 K (the value at 287.32 K was omitted from the smoothed data treatment): $\ln x_1 = -8.6578 + 15.1456/(T/100\ \mathrm{K})$.
The standard error about the regression line is 2.97×10^{-3} and the smoothed data are:

T/K	$10^3 x_1$
278.15	4.067
288.15	3.332
298.15	2.793

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2, evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilibration is attained within 24 h.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be minimum purity of 99 mol %, further purified by sublimation.
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane. Allied Chemical Co. Genetron 113. Dried over Drierite and distilled.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.002$ (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 : [2551-62-4]
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]

Original Measurements:
H. Hiraoka and J. H. Hildebrand, J. Phys. Chem. **68**, 213–214 (1964).

Variables:
T/K = 277.20–308.13
p/kPa = 101.325

Prepared By:
M. E. Derrick and H. L. Clever

Experimental Values

t/°C	T/K	$10^2 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
4.05	277.20	4.166	8.38	8.50
14.97	288.12	3.419	6.71	7.08
24.98	298.13	2.941	5.66	6.18
34.98	308.13	2.613	4.94	5.57

The Bunsen and Ostwald coefficients were calculated by the compilers assuming an ideal gas and Henry's law behavior.
Smoothed Data for use between 278.06 K and 308.35 K: $\ln x_1 = -7.8516 + 12.9269/(T/100\ \mathrm{K})$.
The standard error about the regression line is 5.03×10^{-4} and the smoothed data are:

T/K	$10^2 x_1$
278.15	4.059
288.15	3.455
298.15	2.972
308.15	2.582

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet and a reservoir for the solvent. The buret is thermostated at 25 °C, the pipet from any temperature between 5 °C and 30 °C. The pipet contains a magnetic stirring bar. The pure solvent is degassed by freezing with liquid N_2, evacuating, then boiling with a heat lamp. The process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. The solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by Hg. Its volume is the difference between the capacity of the pipet and the volume of Hg that confines it. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements in the buret before and after introduction of the gas into the buret. With stirring, equilibration is attained in 24 h.

Source and Purity of Material:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be 99%. Purified further by multiple trap sublimation at dry ice alcohol temperatures.
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane. Union Carbide Co. Distilled, purity checked by UV absorbance.

Estimated Error:
δT/K = 0.02
$\delta x_1 / x_1 = 0.003$

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) R-113 or 1,1,2-trichloro-1,2,2-trifluoroethane; CCl_2FCClF_2 ; [76-13-1]

Original Measurements:

H. Jester and P. G. Kosky, J. Chem. Eng. Data **21**, 66–71 (1976).

Variables:

T/K = 233.1–329.0
P_{tot} /MPa = 0.00920–0.2068
Gas mole ratio, n_1/n_2 = 0.0092, 0.0226, and 0.0306

Prepared By:

H. L. Clever

Experimental Values

Vapor+Liquid Mole and Mole Ratio (n/mol cm^{-3})	T/K	Total Pressure (p_{tot} /Torr)	Solvent Pressure (p_2 /Torr)	x_1	Henry's Constant ($10^{-3}H$/Torr)	Henry's Constant (H/MPa)
	233.1	77.6	12.7	0.0063	10.3	1.37
	244.5	95.7	25.3	0.0062	11.3	1.51
$n_1 = 1.26\times10^{-5}$	255.2	126.7	46.3	0.0060	13.4	1.79
$n_2 = 1.37\times10^{-3}$	292.5	418.4	265.9	0.0040	38.1	5.08
$n_1/n_2 = 0.00920$	293.5	418.9	276.3	0.0044	32.4	4.32
	295.4	449.9	298.2	0.0041	37.0	4.93
	319.0	885.9	719.2	0.0041	40.7	5.43
	328.6	1176.5	990.9	0.0038	48.8	6.51
	235.7	171.2	14.9	0.0157	9.95	1.33
$n_1 = 3.09\times10^{-5}$	249.2	233.8	33.4	0.0144	13.9	1.85
$n_2 = 1.37\times10^{-3}$	264.3	337.7	74.0	0.0126	20.9	2.79
$n_1/n_2 = 0.0226$	291.0	609.2	250.0	0.0104	34.5	4.60
	296.7	713.7	314.5	0.0094	42.5	4.60
	312.8	992.9	576.0	0.0097	43.0	5.73
	238.4	238.9	17.6	0.0209	10.6	1.41
	249.5	303.1	33.2	0.0195	13.8	1.84
$n_1 = 4.19\times10^{-5}$	266.9	444.8	84.5	0.0170	21.2	2.83
$n_2 = 1.37\times10^{-3}$	290.4	734.3	244.0	0.0140	35.0	4.67
$n_1/n_2 = 0.0306$	294.9	817.1	292.9	0.0132	39.7	5.29
	312.0	1148.1	559.1	0.0123	47.9	6.39
	328.6	1551.4	989.1	0.0142	39.6	5.28
	329.0	1545.8	998.8	0.0147	37.1	4.95

The authors fitted the Henry's constants, H/Torr = $(p_1$ /Torr$)/x_1$, to the equation:

$$H/\text{Torr} = 9.98\times10^{-9}(T/\text{K})^{5.05} \text{ for } 373\text{ K} > T > 235\text{ K}.$$

The SF_6 vapor pressure was taken as the difference in the total pressure and solvent pressure, $p_1 = (p_{tot} - p_2)$.

Auxiliary Information

Method/Apparatus/Procedure:

See the author's data sheet on $SF_6 + C_6F_{16}$ (Isomeric mixture of perfluorohexanes) for the complete Auxiliary Information.

Source and Purity of Material:

(1) Sulfur hexafluoride. Nothing specified.
(2) R-113. Source and Purity not given. The authors give equations for vapor pressure and density.
$\ln(p_2/\text{Torr}) = -3396.8/(T/\text{K}) + 17.19$
$(\rho/\text{g cm}^{-3}) = 2.24 - 0.0023(T/\text{K})$. The solvent mole wt is 187 and the solubility parameter 7.25 (cal cm^{-3})$^{1/2}$.

Estimated Error:

Nothing specified.

Components:

(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) R-114 or 1,2-dichloro-1,1,2,2-tetrafluoroethane; $CClF_2CClF_2$; [76-14-2]

Original Measurements:

H. Jester and P. G. Kosky, J. Chem. Eng. Data **21**, 66–71 (1976).

Variables:

T/K = 252.0–277.6
P_{tot} /MPa = 0.04210–0.1144
Gas mole ratio, n_1/n_2 = 0.0136

Prepared By:

H. L. Clever

Experimental Values

Vapor+Liquid Mole and Mole Ratio (n/mol cm^{-3})	T/K	Total Pressure (p_{tot} /Torr)	Solvent Pressure (p_2 /Torr)	x_1	Henry's Constant ($10^{-3}H$/Torr)	Henry's Constant (H/MPa)
$n_1 = 1.16\times10^{-5}$	252.0	315.8	261.0	0.0101	5.43	0.724
$n_2 = 8.56\times10^{-4}$	270.8	651.8	596.0	0.0106	5.27	0.703
$n_1/n_2 = 0.0136$	277.6	858.1	783.5	0.0097	7.69	1.025

Henry's constants is H/Torr = $(p_1$ /Torr$)/x_1$.

The SF_6 vapor pressure was taken as the difference in the total pressure and solvent pressure, $p_1 = (p_{tot} - p_2)$.

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus consisted of a 1 L test cell in a thermostat which could be controlled at temperatures between 235 and 373 K. The test cell was connected through a hermetically sealed copper pipe to a 1 L gas measuring volume, a pressure transducer and a vacuum and pressure source. The system was evacuated, the test cell filled with a known volume of solvent and the gas measuring cell filled with SF_6 to a known pressure. The vapor pressure of the solvent was measured in the apparatus. A known amount of gas was added to the test cell. The moles of gas were calculated from the T, and the initial and final p assuming ideal gas behavior. The test cell contents were stirred by a Teflon coated magnetic rod until the equilibrium total pressure, p_{tot} was reached. It was assumed that the vapor-gas mixture obeyed Dalton's law and the ideal gas law and the liquid $\Delta V = 0$.

Source and Purity of Material:

(1) Sulfur hexafluoride. Nothing specified.
(2) R-114. Source and purity not given. Authors gave equations for the solvent vapor pressure and density. $\ln(p_2/\text{Torr}) = -3010.1/(T/\text{K}) + 17.51$ and $(\rho/\text{g cm}^{-3}) = 2.29 - 0.0028(T/\text{K})$. Mol. wt 171, Solubility parameter 8.58 (cal cm^{-3})$^{1/2}$.

Estimated Error:

The authors made no estimate of error.

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Perfuorohexane, isomeric mixture; C_6F_{14}

Original Measurements:
H. Jester and P. G. Kosky, J. Chem. Eng. Data **21**, 66–71 (1976).

Variables:
T/K = 223.9–333.3
P_{tot} /MPa = 0.00448–0.1306
Gas mole ratio, n_1/n_2 = 0.0201, 0.0466

Prepared By:
H. L. Clever

Experimental Values

Vapor+Liquid Mole and Mole Ratio (n/mol cm^{-3})	T/K	Total Pressure (p_{tot} /Torr)	Solvent Pressure (p_2 /Torr)	x_1	Henry's Constant ($10^{-3}H$/Torr)	Henry's Constant (H/MPa)
	223.9	33.6	3.2	0.0173	1.75	0.233
$n_1 = 1.32\times10^{-5}$	247.0	68.8	15.6	0.0156	3.41	0.455
$n_2 = 6.57\times10^{-3}$	273.8	175.3	69.2	0.0120	8.84	1.179
$n_1/n_2 = 0.0201$	295.3	307.7	188.3	0.0117	10.2	1.36
	333.3	980.0	803.2	0.0094	18.9	2.52
$n_1 = 3.06\times10^{-5}$	232.9	94.1	6.2	0.0380	2.31	0.308
$n_2 = 6.57\times10^{-3}$	251.9	178.4	21.0	0.0330	4.77	0.636
$n_1/n_2 = 0.0466$	293.4	483.5	173.2	0.0244	12.7	1.69
	322.8	972.2	554.2	0.0200	20.9	2.79

The authors fitted the Henry's constants, H/Torr = $(p_1$ /Torr$)/x_1$, to the equation:

$$H/\text{Torr} = 4.50\times10^{-15}(T/\text{K})^{7.47} \text{ for } 373\text{ K} > T > 235\text{ K}.$$

The SF_6 vapor pressure was taken as the difference in the total pressure and solvent pressure, $p_1 = (p_{tot} - p_2)$.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consisted of a 1 L test cell in a thermostat which could be controlled at temperatures between 235 and 373 K. The test cell was connected through a hermetically sealed copper pipe to a 1 L gas measuring volume, a pressure transducer and a vacuum and pressure source. The system was evacuated, the test cell filled with a known volume of solvent and the gas measuring cell filled with SF_6 to a known pressure. The vapor pressure of the solvent was measured in the apparatus. A known amount of gas was added to the test cell. The moles of gas were calculated from the T, and the initial and final p assuming ideal gas behavior. The test cell contents were stirred by a Teflon coated magnetic rod until the equilibrium total pressure, p_{tot} was reached. It was assumed that the vapor-gas mixture obeyed Daltons law and the ideal gas law and the liquid $\Delta V = 0$.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Nothing specified.
(2) Perfluorohexane Isomer Mixture. Stated to be 54% 2,3-dimethylbutane, 39% 2-methylpentane, and 7% hexane. Authors gave equations for the solvent vapor pressure and density.
$\ln(p_2/\text{Torr}) = -3758.5/(T/\text{K}) + 17.96$, and $(\rho/\text{g cm}^{-3}) = 2.60 - 0.0029(T/\text{K})$. Mol. wt 338, Solubility parameter is 5.93 (cal cm^{-3})$^{1/2}$.

Estimated Error:
The authors made no estimate of error. The fact that temperature and Henry's constant fell on a common lg-lg plot at several n_1/n_2 ratios was taken to mean Henry's constant was independent of pressure.

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) FC-82 or Decafluorobis(trifluoromethyl)-cyclohexane; C_8F_{16} ; [26637-68-3]

Original Measurements:
H. Jester and P. G. Kosky, J. Chem. Eng. Data **21**, 66–71 (1976).

Variables:
T/K = 238.6–373.6
P_{tot} /MPa = 0.00719–0.2061
Gas mole ratio, n_1/n_2 = 0.0211, 0.1047

Prepared By:
H. L. Clever

Experimental Values

Vapor+Liquid Mole and Mole Ratio (n/mol cm^{-3})	T/K	Total Pressure (p_{tot} /Torr)	Solvent Pressure (p_2 /Torr)	x_1	Henry's Constant ($10^{-3}H$/Torr)	Henry's Constant (H/MPa)
	238.6	53.9	1.4	0.016	3.28	0.437
	247.0	57.5	2.6	0.016	3.43	0.457
	255.3	67.4	4.6	0.0155	4.05	0.540
	264.3	87.2	7.8	0.0144	5.51	0.735
$n_1 = 1.34\times10^{-5}$	276.6	111.4	15.8	0.0134	7.14	0.952
$n_2 = 6.35\times10^{-4}$	288.5	148.0	29.4	0.0121	9.80	1.307
$n_1/n_2 = 0.0211$	301.9	190.3	55.9	0.0114	11.8	1.573
	306.1	229.3	67.9	0.0096	16.8	2.24
	316.4	291.4	105.4	0.0084	22.1	2.95
	328.0	370.2	168.6	0.0079	25.5	3.40
	339.7	483.4	261.0	0.0071	31.3	4.17
	350.6	620.9	382.4	0.0067	35.6	4.75
	362.0	816.5	557.5	0.0060	43.2	5.76
	373.6	1069.1	796.4	0.0058	47.0	6.27
	238.8	233.6	1.4	0.0772	3.00	0.400
	247.0	274.8	2.6	0.0748	3.64	0.485
	255.4	334.2	4.5	0.0713	4.62	0.616
$n_1 = 6.65\times10^{-5}$	266.5	454.0	9.0	0.0641	6.94	0.925
$n_1 = 6.65\times10^{-5}$	277.5	560.5	16.6	0.0587	9.27	1.236
$n_1/n_2 = 0.1047$	295.3	739.3	41.1	0.0510	13.7	1.83
	296.7	753.8	43.9	0.0505	14.1	1.88
	297.3	769.1	43.9	0.0497	14.6	1.95
	320.6	1047.3	125.4	0.0381	24.2	3.23
	351.5	1546.1	394.9	0.0343	33.6	4.484

The authors fitted the Henry's constants, H/Torr = $(p_1$ /Torr$)/x_1$, to the equation:

$$H/\text{Torr} = 4.82\times10^{-12}(T/\text{K})^{6.23} \text{ for } 373\text{ K} > T > 235\text{ K}.$$

The SF_6 vapor pressure was taken as the difference in the total pressure and solvent pressure, $p_1 = (p_{tot} - p_2)$.

Auxiliary Information

Method/Apparatus/Procedure:
For the complete auxiliary information see the author's data sheet for $SF_6 + C_6F_{14}$. Isomeric mixture of perfluorohexanes.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Nothing specified.
(2) FC-82. Minnesota Minning & Manufacturing Co. Authors gave equations for the solvent vapor pressure and density.
$\ln(p_2/\text{Torr}) = -4176.9/(T/\text{K}) + 17.86$ and $(\rho/\text{g cm}^{-3}) = 2.55 - 0.0024(T/\text{K})$. Mol. wt 400, Solubility parameter is 6.17 (cal cm^{-3})$^{1/2}$.

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) FC-88. See source below.

Original Measurements:
H. Jester and P. G. Kosky, J. Chem. Eng. Data **21**, 66–71 (1976).

Variables:
T/K = 238.6–320.5
P_{tot} /MPa = 0.01979–0.2261
Gas mole ratio, n_1/n_2 = 0.0237, 0.0635

Prepared By:
H. L. Clever

Experimental Values

Vapor+Liquid Mole and Mole Ratio (n/mol cm^{-3})	T/K	Total Pressure (p_{tot} /Torr)	Solvent Pressure (p_2 /Torr)	x_1	Henry's Constant ($10^{-3}H$/Torr)	Henry's Constant (H/MPa)
$n_1 = 1.29\times10^{-5}$	297.0	729.2	604.2	0.0138	9.20	1.227
$n_2 = 5.45\times10^{-4}$	304.9	1065.3	910.6	0.0123	12.6	1.68
$n_1/n_2 = 0.0237$	312.7	1209.1	1052.4	0.0125	12.5	1.67
	320.5	1695.8	1528.2	0.0123	13.6	1.81
	238.6	148.4	39.6	0.0532	2.05	0.273
	255.4	265.3	97.8	0.0487	3.44	0.459
	270.9	436.5	206.0	0.0444	5.19	0.692
	290.2	791.6	463.5	0.0385	8.51	1.135
$n_1 = 3{,}46\times10^{-5}$	292.5	853.3	507.5	0.0373	9.27	1.236
$n_2 = 5.45\times10^{-4}$	296.3	937.1	586.3	0.0376	9.33	1.244
$n_1/n_2 = 0.0635$	296.4	919.5	587.5	0.0392	8.47	1.129
	296.5	936.0	589.9	0.0380	9.11	1.215
	296.6	954.1	592.4	0.0367	9.86	1.315
	296.8	959.3	596.1	0.0366	9.92	1.323
	305.5	1205.0	821.2	0.0366	10.5	1.40
	315.0	1205.0	1138.3	0.0380	10.3	1.37

The authors fitted the Henry's constants, $H/\text{Torr} = (p_1/\text{Torr})/x_1$, to the equation:

$$H/\text{Torr} = 1.68\times10^{-12}(T/\text{K})^{6.35} \text{ for } 373\text{ K} > T > 235\text{ K}.$$

The SF_6 vapor pressure was taken as the difference in the total pressure and solvent pressure, $p_1 = (p_{tot} - p_2)$.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consisted of a 1 L test cell in a thermostat which could be controlled at temperatures between 235 and 373 K. The test cell was connected through a hermetically sealed copper pipe to a 1 L gas measuring volume, a pressure transducer and a vacuum and pressure source. The system was evacuated, the test cell filled with a known volume of solvent and the gas measuring cell filled with SF_6 to a known pressure. The vapor pressure of the solvent was measured in the apparatus. A known amount of gas was added to the test cell. The moles of gas were calculated from the T, and the initial and final p assuming ideal gas behavior. The test cell contents were stirred by a Teflon coated magnetic rod until the equilibrium total pressure, p_{tot} was reached.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Nothing specified.
(2) FC-88. Minnesota Mining & Manufacturing Co. No information. See "Fluorine Electronic Liquids" Catalogues, 3M, St Paul, MN. Authors gave equations for the solvent vapor pressure and density.
$\ln(p_2/\text{Torr}) = -3308.5/(T/\text{K}) + 17.54$ and $(\rho/\text{g cm}^{-3}) = 2.39 - 0.0025(T/\text{K})$. Mol. wt 300,
Solubility parameter is 5.81 (cal cm^{-3})$^{1/2}$.

Estimated Error:
The authors made no estimate of error. The fact that temperature and Henry's constant fell on a common lg-lg plot at several n_1/n_2 ratios was taken to mean Henry's constant was independent of pressure.

Components:
(1) Sulfur fluoride or sulfur hexafluoride, SF_6; [2551-62-4]
(2) FC-75 or Fluorinert or perfluoro-2-butyl-tetrahydrofuran; $C_8F_{16}O$; [11072-16-5]

Original Measurements:
H. Jester and P. G. Kosky, J. Chem. Eng. Data **21**, 66–71 (1976).

Variables:
T/K = 239.3–370.1
P_{tot} /MPa = 0.00673–0.1841
Gas mole ratio, n_1/n_2 = 0.0283, 0.0525, and 0.1221

Prepared By:
H. L. Clever

Experimental Values

Vapor+Liquid Mole and Mole Ratio (n/mol cm^{-3})	T/K	Total Pressure (p_{tot} /Torr)	Solvent Pressure (p_2 /Torr)	x_1	Henry's Constant ($10^{-3}H$/Torr)	Henry's Constant (H/MPa)
	239.3	50.5	0.9	0.0232	2.14	0.285
$n_1 = 1.61\times10^{-5}$	272.0	130.6	8.1	0.0174	7.04	0.939
$n_2 = 5.69\times10^{-4}$	293.8	201.5	26.7	0.0139	12.6	1.68
$n_1/n_2 = 0.0283$	294.7	196.2	28.0	0.0145	11.6	1.55
	338.3	457.7	191.7	0.0095	28.0	3.73
	247.9	134.0	1.7	0.0388	3.40	0.453
	268.1	199.4	6.4	0.0345	5.59	0.745
$n_1 = 2.99\times10^{-5}$	277.2	246.9	10.9	0.0314	7.52	1.003
$n_2 = 5.69\times10^{-4}$	296.5	359.7	20.7	0.0254	13.0	1.73
$n_1/n_2 = 0.0525$	313.1	471.5	67.2	0.0213	19.0	2.53
	353.6	890.3	336.9	0.0153	36.2	4.83
	370.1	1154.0	586.5	0.0165	34.4	4.59
	239.5	247.6	0.9	0.0900	2.74	0.365
$n_1 = 6.95\times10^{-5}$	253.1	361.1	2.4	0.0819	4.38	0.584
$n_2 = 5.59\times10^{-4}$	298.4	810.7	33.7	0.0566	13.7	1.83
$n_1/n_2 = 0.1221$	325.1	1149.0	113.2	0.0441	23.5	3.13
	344.6	1380.9	243.9	0.0422	26.9	3.59

The authors fitted the Henry's constants, $H/\text{Torr} = (p_1/\text{Torr})/x_1$, to the equation:

$$H/\text{Torr} = 1.41\times10^{-12}(T/\text{K})^{6.43} \text{ for } 373\text{ K} > T > 235\text{ K}.$$

The SF_6 vapor pressure was taken as the difference in the total pressure and solvent pressure, $p_1 = (p_{tot} - p_2)$.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consisted of a 1 L test cell in a thermostat which could be controlled at temperatures between 235 and 373 K. The test cell was connected through a hermetically sealed copper pipe to a 1 L gas measuring volume, a pressure transducer and a vacuum and pressure source. The system was evacuated, the test cell filled with a known volume of solvent and the gas measuring cell filled with SF_6 to a known pressure. The vapor pressure of the solvent was measured in the apparatus. A known amount of gas was added to the test cell. The moles of gas were calculated from the T, and the initial and final p assuming ideal gas behavior. The test cell contents were stirred.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Nothing specified.
(2) FC-75. Minnesota Mining & Manufacturing Co. Perfluoro-2-butyl-tetrahydrofuran, 95 mole %. Authors gave equations for the solvent vapor pressure and density.
$\ln(p_2/\text{Torr}) = -4398.9/(T/\text{K}) + 18.26$ and $(\rho/\text{g cm}^{-3}) = 2.48 - 0.0024(T/\text{K})$. Mol. wt is 416,
Solubility parameter is 6.24 (cal cm^{-3})$^{1/2}$.

Estimated Error:
The authors made no estimate of error. The fact that temperature and Henry's constant fell on a common lg-lg plot at several n_1/n_2 ratios was taken to mean Henry's constant was independent of p.

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Bromocyclohexane; $C_6H_{11}Br$; [108-85-0]

Original Measurements:
M. C. Lopez, M. A. Gallardo, J. S. Urieta, and C. Gutierrez, J. Chem. Eng. Data **32**, 472–474 (1989).

Variables:
T/K = 263.15–303.15
p_1 /bar = 1.013

Prepared By:
C. L. Young

Experimental Values

T/K	$10^4 x_1$
263.15	25.3
273.15	23.4
283.15	21.9
293.15	20.6
303.15	19.5

The authors fitted the data to the equation: $\ln x_1 = -15.7884 + [855.0286/(T/\mathrm{K})] + 1.1771 \ln(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility apparatus was similar to that used by Ben-Naim and Baer[1] consisting essentially of a gas buret, mercury manometer, and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It was assumed that the mole fraction of the solvent was that corresponding to the vapor pressure of the pure solvent. It appears that the mole fraction at a partial pressure of 1 atm was estimated from raw experimental data assuming Henry's law is obeyed.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Sociedad Espanola del Oxigene, S.A. Purity stated to be 99.5 mole %.
(2) Bromocyclohexane. Fluka. Purity 99+mole% as determined by gas chromatography.

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.015

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 : [2551-62-4]
(2) Carbon disulfide; CS_2 ; [75-15-0]

Original Measurements:
R. J. Powell, J. Chem. Eng. Data **17**, 302–304 (1971).

Variables:
T/K = 272.15–303.15
p/kPa = 101.325

Prepared By:
P. L. Long and H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})	Slope (N) = ($R\Delta \log x_1 / \Delta \log T$)*
298.15	8.12	0.300	0.328	0.00

The Bunsen and Ostwald coefficients were calculated by the compilers assuming an ideal gas and Henry's law behavior.
*The author states that the solubility measurements were made over the temperature interval of about 273.15–303.15 K. Only the solubility value of 298.15 K was given in the paper. The slope, $N = R[\Delta \log x_1 / \Delta \log(T/\mathrm{K})] = 0.00$ which implies that the mole fraction solubility at 1 atm is the same, within experimental error, over the temperature interval of the measurements.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is the Diamond and Hildebrand[1] apparatus which uses an all glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final pressures. The solvent is degassed by freezing, pumping and followed by boiling under reduced pressure.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Source not given. Stated to be manufacturer's research grade, dried over $CaCl_2$ before use.
(2) Carbon disulfide. Source not given. Stated to be manufacturer's spectrochemical grade.

Estimated Error:
$\delta x_1 / x_1$ = ±0.002
δN/cal K^{-1} mol^{-1} = ±0.1

References:
[1]J. H. Diamond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 : [2551-62-4]
(2) Carbon disulfide; CS_2 ; [75-15-0]

Original Measurements:
Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331–335 (1961).

Variables:
T/K = 288.29–303.65
p/kPa = 101.325

Prepared By:
M. E. Derrick and H. L. Clever

Experimental Values

t/°C	T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^{3}cm^{-3})
15.14	288.29	9.23	0.345	0.364
20.12	293.27	9.20	0.342	0.367
25.00*	298.15*	9.245	0.342	0.373
25.45	298.60	9.237	0.342	0.374
30.13	303.28	9.18	0.338	0.375
30.50	303.65	9.222	0.339	0.377

*The 298.15 K value may be a smoothed value of the authors.

The Bunsen and Ostwald coefficients were calculated by the compilers assuming an ideal gas and Henry's law behavior. Smoothed Data for use between 288.29 K and 303.65 K: $\ln x_1 = -7.0233 + 0.1019/(T/100\ \mathrm{K})$.
The standard error about the regression line is 2.65×10^{-6}, and smoothed solubility data are:

T/K	$10^4 x_1$
288.15	9.23
293.15	9.22
298.15	9.22
303.15	9.21

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C, the pipet from any temperature between 5 and 30 °C. The pipet contains a magnetic stirring bar. The pure solvent is degassed by freezing with liquid N_2, evacuating, then boiling with a heat lamp. The process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. The solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by Hg. Its volume is the difference between the capacity of the pipet and the volume of Hg that confines it. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements in the buret before and after introduction of the gas into the buret. With stirring, equilibration is attained in 24 h.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be 99%. Purified further by multiple trap sublimation at dry ice alcohol temperatures.
(2) Carbon disulfide. Mallinckrodt Chemical Works. Analytical Reagent grade. Shaken successively with Hg and $HgCl_2$, filtered, distilled, and stored over Hg more than 5 days before use.

Estimated Error:
δT/K = 0.02
$\delta x_1 / x_1 = 0.003$

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Sulfinylbismethane or dimethylsulfoxide; C_2H_6OS; [67-68-5]

Original Measurements:
N. Brückl and J. I. Kim, Z. Phys. Chem. (Wiesbaden) **133**, 133–150 (1981).

Variables:
T/K = 298.2
p_t /MPa = 0.1013

Prepared By:
C. L. Young

Experimental Values
The solubility of sulfur hexafluoride in dimethylsulfoxide at 298.2 K and a partial pressure of 0.1013 MPa

T/K	Henry's Constant [$\ln(K_H$ /atm)]	Mole Fraction $10^3 x_1$
298.2	8.52	0.1994

The compiler calculated the mole fraction solubility at a partial pressure of 1 atm (0.1013 MPa) assuming $x_1 = 1/K_H$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by a volumetric method described as "the Ostwald method." No other details given.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Linde Co. Purity stated to be 99.8 volume%.
(2) Dimethylsulfoxide. Uvasol or analytical grade.

Estimated Error:
δT/K = ±0.1
δK_H = ±1.25%

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Nitrogen oxide; N_2O_4 ; [10544-72-6]

Original Measurements:
E. T. Chang, N. A. Gocken, and T. M. Poston, J. Chem. Eng. Data **16**, 404–408 (1971).

Variables:
T/K = 263.15, 278.13, and 293.14
P_1 /kPa = 44.52–141.42

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

The solubility of sulfur hexafluoride in liquid N_2O_4

T/K	Partial Pressure (p_1 /atm)	Partial Pressure (p_1 /kPa)	Solubility 10^3x_1
263.15	0.7095	71.89	8.179
263.15	1.3778	139.61	16.48
278.13	0.6635	67.23	6.427
278.13	1.3957	141.42	13.96
293.14	0.4394	44.52	3.643
293.14	0.9478	96.04	8.013
293.14	1.1006	111.52	9.346

Auxiliary Information

Method/Apparatus/Procedure:
A volumetric apparatus consisting of solvent vessel and buret with three calibrated bulbs. Pressure changes measured with mercury manometer and cathetometer. Solvent stirred with magnet enclosed in glass. Mole fraction absorbed calculated from knowledge of amount of solute gas before and after absorption. Solvent carefully degassed.

Source and Purity of Materials:
(1) Sulfur hexafluoride. A sample of 98.7 mole %, frozen in liquid nitrogen and 1.1 mole % air removed.
(2) Nitrogen oxide. Research grade gas. Purity stated to be 99.5 mole % minimum, further purified by bubbling oxygen through, degassed distilled.

Estimated Error:
δT/K = ±0.1
δp_1 /kPa = ±0.01
δx_1 /x_1 = ±0.02

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Nitromethane; CH_3NO_2 ; [75-52-5]

Original Measurements:
H. L. Friedman, J. Am. Chem. Soc. **76**, 3294–3297 (1954).

Variables:
T/K = 273.25, 292.50, and 298.00
p_1 /kPa = 93.33 (700 mmHg)

Prepared By:
H. L. Clever

Experimental Values

The solubility of sulfur hexafluoride in nitromethane

t/°C	T/K	Ostwald Coefficeint (L/cm^3 cm^{-3})	10^5x_1	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]
0.1	273.25	0.374		
0.1	273.25	0.369		
0.1	273.25	Av. 0.372	86.8	0.372
19.35	292.50	0.354		
19.35	292.50	0.364		
19.35	292.50	0.369		
		Av. 0.363	81.7	0.344
24.85	298.00	0.374		
24.85	298.00	0.380		
24.85	298.00	Av. 0.377	83.1	83.1

The compiler calculated and added the Kelvin temperature, the Bunsen coefficient and mole fraction values. The solubility calculations were made for a partial pressure of 101.325 kPa (760 mmHg) assuming Henry's law and ideal gas behavior.

Auxiliary Information

Method/Apparatus/Procedure:
The gas absorption method was essentially that employed by Euken and Herzberg.[1] Their method was modified by the use of a magnetic stirrer, and by use of electrical contacts in the mercury manometer to aid balancing the pressure.
The solvent was degassed by vacuum. The procedure, repeated 5–10 times, was to alternate 5–15 s evacuation with rapid stirring to produce cavitation. In the solubility measurement, gas presaturated with solvent vapor, was brought into contact with about 80 cm^3 of solvent in the saturation vessel. Initial conditions were established by a time extrapolation. Solubility was approached from both under- and super-saturation.
See also the data sheet of sulfur hexafluoride+water from this paper.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Fractionally condensed at 83.15 K. Vapor pressure 275–6 mmHg at 195.15 K agrees with literature value.[2]
(2) Nitromethane. Source not given. Dried by filtering at 253 K, distilled.

Estimated Error:
δT/K = ±0.05
δp_1 /mmHg = ±0.3
$\delta L/L$ = ±0.03

References:
[1]A. Euken and G. Herzberg, Z. Phys. Chem. **1**, 195 (1950).
[2]W. C. Schumb, Ind. Eng. Chem. **39**, 421 (1947).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Methylhydrazine; $N_2H_3CH_3$; [60-34-4]

Original Measurements:
E. T. Chang, N. A. Gocken, and T. M. Poston, J. Chem. Eng. Data **16**, 404–408 (1971).

Variables:
T/K = 253.7–313.23
P_1 /kPa = 23.68–220.55

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

The solubility of sulfur hexafluoride in liquid $N_2H_3CH_3$

T/K	Partial Pressure (p_1 /atm)	Partial Pressure (p_1 /kPa)	10^3x_1
253.7	0.2337	23.68	0.052
253.7	0.3233	32.76	0.072
253.7	0.9890	100.21	0.218
253.7	1.0524	106.63	0.232
253.7	1.9580	198.39	0.428
253.7	2.0329	205.98	0.444
273.15	0.5344	54.15	0.111
273.15	0.7783	78.86	0.161
273.15	0.8072	81.79	0.169
273.15	1.0920	110.65	0.228
273.15	2.0802	202.50	0.413
293.14	0.7206	73.01	0.150
293.14	1.0085	102.19	0.211
293.14	1.0815	109.58	0.224
293.14	1.0955	111.00	0.227
293.15	1.9515	197.64	0.416
293.15	1.9557	198.16	0.416
293.15	2.1767	220.55	0.448
313.23	0.9514	96.40	0.185
313.23	1.7330	175.60	0.347

Auxiliary Information

Method/Apparatus/Procedure:
A volumetric apparatus consisting of solvent vessel and buret with three calibrated bulbs. Pressure changes measured with mercury manometer and cathetometer. Solvent stirred with magnet enclosed in glass. Mole fraction absorbed calculated from knowledge of amount of solute gas before and after absorption. Solvent carefully degassed.

Source and Purity of Materials:
(1) Sulfur hexafluoride. A sample of 98.7 mole %, frozen in liquid nitrogen and 1.1 mole % air removed.
(2) Methylhydrazine. A sample of purity 99 mole % further purified by double vacuum distillation.

Estimated Error:
δT/K = ±0.1
δp_1 /kPa = ±0.01
$\delta x_1 / x_1 = <\pm 0.02$

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Hexamethylphosphoric triamide; $C_6H_{18}NO_3P$; [680-31-9]

Original Measurements:
N. Brückl and J. I. Kim, Z. Phys. Chem. (Wiesbaden) **133**, 133–150 (1981).

Variables:
T/K = 298.2
p_t /MPa = 0.1013

Prepared By:
C. L. Young

Experimental Values

T/K	Henry's Constant $\ln(K_H$ /atm)	10^3x_1
298.2	6.05	2.36

The compiler calculated the mole fraction solubility at a partial pressure of 1 atm (0.1013 MPa) assuming $x_1 = 1/K_H$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility were determined by a volumetric method described as the ''Ostwald method.'' No other details given.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Linde Co. Purity stated to be 99.8 volume%.
(2) Hexamethylphosphoric triamide. Uvasol or analytical grade.

Estimated Error:
δT/K = ±0.1
δK_H = ±1.25%

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Benzonitrile; C_7H_5N; [100-47-0]
(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]
(2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

Original Measurements:
N. Brückl and J. I. Kim, Z. Phys. Chem. (Wiesbaden) **133**, 133–150 (1981).

Variables:
T/K = 298.2
p_t /MPa = 0.1013

Prepared By:
C. L. Young

Experimental Values

Solvent and T/K	Henry's Constant [ln(K_H /atm)]	$10^3 x_1$
Benzonitrile: 298.2	6.67	1.268
1,4-Dioxane: 298.2	6.53	1.459
Nitrobenzene: 298.2	6.98	0.930

The compiler calculated the mole fraction solubility at a partial pressure of 1 atm (0.1013 MPa) assuming $x_1 = 1/K_H$.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility were determined by a volumetric method described as "Ostwald method." No other details given.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Linde Co. Purity stated to be 99.8 volume %.
(2) Benzonitrile.
(2) 1,4-Dioxane.
(2) Nitrobenzene.
All Uvasol or analytical grade.

Estimated Error:
δT/K = ±0.1
δK_H = ±1.25%

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) N,N-Dimethylacetamide; C_4H_9NO; [127-19-5]
(2) N,N-Dimethylformamide; C_3H_7NO; [68-12-7]
(2) N-Methylformamide; C_2H_5NO; [123-39-7]
(2) Acetonitrile; C_2H_3N; [75-05-8]

Original Measurements:
N. Brückl and J. I. Kim, Z. Phys. Chem. (Wiesbaden) **133**, 133–150 (1981).

Variables:
T/K = 298.2
p_t /MPa = 0.1013

Prepared By:
C. L. Young

Experimental Values

Solvent	T/K	Henry's Constant [ln(K_H /atm)]	$10^3 x_1$
N,N-Dimethylacetamide:	298.2	6.85	1.059
N,N-Dimethylformamide:	298.2	7.17	1.059
N-Methylformamide:	298.2	7.76	1.059
Acetamide:	298.2	7.76	1.416

The compiler calculated the mole fraction solubility at a partial pressure of 1 atm (0.1013 MPa) assuming $x_1 = 1/K_H$.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined by a volumetric method described as "the Ostwald method." No other details given.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Linde Co. Purity stated to be 99.8 volume %.
(2) N,N-Dimethylacetamide
(2) N,N-Dmethylformamide
(2) N-Methylformamide
(2) Acetamide
All Uvasol or analytical grade.

Estimated Error:
δT/K = ±0.1
δK_H = ±1.25%

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 : [2551-62-4]
(2) 1,1,2,2,3,3,4,4,4-Nonafluoro-*N*,*N*-bis(nonafluorobutyl)-1-butanamine or perfluorotributylamine; $C_{12}F_{27}N$; [311-89-7]

Original Measurements:
H. Hiraoka and J. H. Hildebrand, J. Phys. Chem. **68**, 213–214 (1964).

Variables:
T/K = 278.06–308.35
p/kPa = 101.325

Prepared By:
M. E. Derrick and H. L. Clever

Experimental Values

t/°C	T/K	$10^2 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
4.91	278.06	10.85	7.85	7.99
14.91	288.06	8.88	6.20	6.54
24.96	298.11	7.28	4.93	5.38
35.20	308.35	6.079	4.01	4.53

The compiler calculated the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 278.06 K and 308.35 K: $\ln x_1 = -8.1367 + 16.4531/(T/100\ \text{K})$.
The standard error about the regression line is 2.74×10^{-4} and smoothed solubility data follow.

T/K	$10^2 x_1$
278.15	10.84
288.15	8.83
298.15	7.29
308.15	6.10

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet and a reservoir for the solvent. The buret is thermostated at 25 °C, the pipet from any temperature between 5 and 30 °C. The pipet contains a magnetic stirring bar. The pure solvent is degassed by freezing with liquid N_2, evacuating, then boiling with a heat lamp. The process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. The solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by Hg. Its volume is the difference between the capacity of the pipet and the volume of Hg that confines it. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements in the buret before and after introduction of the gas into the buret. With stirring, equilibration is attained in 24 h.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. Stated to be 99%. Purified further by multiple trap sublimation at dry ice alcohol temperatures.
(2) Perfluorotributylamine. Minnesota Mining and Manufacturing Co. Dried, fractionated, boiling point 178.5–179.0 °C. Density at 298.15 K, $\rho = 1.872$ g cm^{-3}.

Estimated Error:
δT/K = 0.02
$\delta x_1 / x_1 = 0.003$

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 : [2551-62-4]
(2) 1,1,2,2,3,3,4,4,4-Nonafluoro-*N*,*N*-bis(nonafluorobutyl)-1-butanamine or perfluorotributylamine; $C_{12}F_{27}N$; [311-89-7]

Original Measurements:
R. J. Powell, J. Chem. Eng. Data **17**, 302–304 (1971).

Variables:
T/K = 288.15–318.15
p/kPa = 101.325

Prepared By:
P. L. Long and H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})	Slope N = [$R(\Delta \log x_1 / \Delta \log T)$]
298.15	774.6	5.27	5.75	−11.60

The compiler calculated the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior.
The author states that the solubility measurements were made over the temperature interval of about 288.15–318.15 K. Only the solubility value of 298.15 K was given in the paper. The slope $N = R(\Delta \log x_1 / \Delta \log T)$ was given.
Smoothed data for use between 288.15 K and 318.15 K, the compiler calculated the smoothed data from the author's slope and solubility value at 298.15 K. The slope equation was rearranged to:

$$\lg x_1 = \lg(0.07746) - (11.60/R)\lg[(T/\text{K})/298.15] \quad \text{with} \quad R = 1.9872\ \text{cal K}^{-1}\ \text{mol}^{-1}.$$

T/K	x_1
288.15	0.09453
298.15	0.07746
308.15	0.06389
318.15	0.05303

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is the Diamond and Hildebrand[1] apparatus which uses an all glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final pressures. The solvent is degassed by freezing, pumping and followed by boiling under reduced pressure.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Source not given. Stated to be manufacturer's research grade, dried over $CaCl_2$ before use.
(2) Perfluorotributylamine. Minnesota Mining and Manufacturing Co. Distilled, used portion boiling between 447.85–448.64 K which gave a single GLC peak. Density at 298.15 K, $\rho = 1.880$ g cm^{-3}.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.002$
δN/cal K^{-1} mol^{-1} = ± 0.1

References:
[1]J. H. Diamond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Tetrachlorosilane or silicon tetrachloride; $SiCl_4$; [10026-04-7]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 298.15
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of SF_6 in CCl_4 at partial pressure 0.101325 MPa and 298.15 K

t/°C	T/K	$10^2 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
25.0	298.15	1.428	2.82	3.08

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2 , evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilibration is attained within 24 h.

Source and Purity of Materials:
(1) Tetrafluoromethane. Matheson Co., Inc. Stated to be minimum purity of 95 mol %, further purified by multiple trap distilltion.
(2) Tetrachlorosilane. Dried over Drierite and distilled.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.002$ (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Tetramethylsilane; $C_4H_{12}Si$; [75-76-3]

Original Measurements:
L. E. W. Horsman-van den Dool and J. W. Warman, Interuniversity Reactor Institute (IRI)-Report 134-81-01.

Variables:
T/K = 291.4
P_1 /kPa = not given.

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	Ostwald Coefficient (L/cm^3 cm^{-3})	Number of Runs
18.2	291.4	3.61	3

Auxiliary Information

Method/Apparatus/Procedure:
A cylindrical glass container of approximately 15 cm^3 volume is filled with solvent and closed with a half-hole septum. An amount of gaseous solute is added to the container. The closed container is shaken for 30 min. Samples of both the vapor and liquid phases are taken in calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.
The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 20 cm Porapack Q column is used for the separation.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Baker Chemical Co. Instrument Grade, 99.9%. Used as received.
(2) Tetramethylsilane. Merck, Uvasol grade. Impurities which give the same retention time as the solute gas are removed before the experiment by absorption or distillation.

Estimated Error:
$\delta L / L = \pm 0.05$

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Octamethylcyclotetrasiloxane; $C_8H_{24}O_4Si_4$; [556-67-2]

Original Measurements:
R. J. Wilcock, J. L. McHale, R. Battino, and E. Wilhelm, Fluid Phase Equilib. **2**, 225–230 (1978).

Variables:
T/K = 292.15–313.16
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	10^2x_1	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
292.15	2.083	1.520	1.626
298.40	1.918	1.388	1.516
313.16	1.664	1.182	1.355

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 292.15 K and 313.15 K: $\ln x_1 = -7.1800 + 9.6505/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.94×10^{-4} and smoothed solubility data follow.

T/K	10^2x_1
298.15	1.938
313.15	1.745

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.8 mol %.
(2) Octamethylcyclotetrasiloxane. General Electric Co. Distilled, density at 298.15 K, ρ/g cm^{-3} = 0.9500.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.1

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Human lung homogenate

Original Measurements:
L. Cander, J. Appl. Physiology **14**, 538–540 (1959).

Variables:
T/K = 310.15

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]
37.0	310.2	0.0074
		0.0064
		0.0063
		0.0069
		Average: 0.0068 ± 0.0005

Auxiliary Information

Procedure/Apparatus/Method:
Solubility was measured with a Van Slyke-Neill apparatus.[1] The homogenized tissue was pressed through several layers of gauze to remove any large shreds of connective tissue. The fluid was deaerated, then equilibrated for 5 m with the gas by shaking. The excess gas was expelled, and the dissolved gas was extracted and its pressure read on a manometer.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Nothing specified.
(2) Human lung homogenate. Lung tissue from deceased patients who had no history of acute or chronic lung disease. The lung was removed, perfused with isotonic saline until blood free, minced, blended, and homogenized.

Error Estimate:
Reproducibility was in the range 2%–9%.

References:
[1]D. D. Van Slyke and J. M. Neill, J. Biol. Chem. **61**, 523 (1924).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Phosphate buffer and human red cell ghosts in phosphate buffer.

Original Measurements:
G. G. Power and H. Stegall, J. Appl. Physiology **29**, 145–149 (1970).

Variables:
T/K = 310.15

Prepared By:
C. L. Young

Experimental Values

Solubility data at 310.15 K

Solvent	Bunsen Coefficient (α/cm^3 cm^{-3} atm^{-1})	Number of Measurements	Standard Deviation
Phosphate Buffer	0.00388	4	0.00002
Ghosts suspended In buffer	0.00475	5	0.00011

The authors calculated the Bunsen Coefficient of SF_6 due to the ghosts by subtracting the phosphate buffer value from the ghost suspension value and dividing by the ghosts per cm^3, i.e.

α° ghost = (α ghost suspension − α buffer)/g ghosts cm^{-3} = 0.151 ± 0.009.

Auxiliary Information

Method/Apparatus/Procedure:
Samples of 5–12 cm^3 were placed in a stirrer cell and gas, saturated with water vapor, passed through the cell for 30–60 min. Samples of the saturated liquid withdrawn and transferred to a Van Slyke apparatus. The dissolved gas removed under reduced pressure. The red cell ghosts were prepared by centrifugation of human blood and lysing the cells using phosphate buffer of pH 7.4. Ghost separated by high speed centrifugation. Washed with phosphate buffer containing 0.01 mol L^{-1} sodium nitrate.

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co., Inc. stated to have a purity of 98 mole % minimum.
(2) See method.

Estimated Error:
δT/K = ±0.1

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Rat abdominal muscle

Original Measurements:
A. Campos Carles, T. Kawashiro, and J. Piiper Pflugers Arch. **359**, 209–218 (1975).

Variables:
T/K = 310.15

Prepared By:
H. L. Clever

Experimental Values

Temperature		Solubility Coefficient /μmol dm^{-3} mmHg^{-1}		Bunsen Coefficient
(t/°C)	(T/K)	Experimental	Corrected	[α/cm^3 (STP) cm^{-3} atm^{-1}]
37	310.15	0.539 ± 0.021	0.559	0.00952

The solubility coefficient is the mean of ten measurements ± the standard error. Correction factors were applied for the unextracted gas and the gas lost during transfer between chambers.

In Kawashiro *et al.*[1] that followed this paper, the authors report diffusion coefficients of SF_6 in rat Skeletal muscle at 37 °C.

Krogh's diffusion constant: 10^9 K/mmol min^{-1} cm^{-1} mmHg^{-1} = 0.081 ± 0.001;

Diffusion coefficient: 10^6 D/cm^2 s^{-1} = 2.41.

Auxiliary Information

Method/Apparatus/Procedure:
The sulfur hexafluoride, saturated with water vapor, was led through an equilibration chamber for 2 h at a rate of 8 ml min^{-1}. The muscle rested on a screen in the equilibration chamber so that it was exposed on all sides. After equilibration the muscle sample was transferred to an extraction chamber filled with room air for the same length of time as the equilibration. The gas in the chamber was forced into a gas chromatograph for analysis by mercury entering the chamber.

Source and Purity of Material:
(1) Sulfur hexafluoride. Stated to be better than 99.9% pure.
(2) Rat abdominal muscle. A flat muscle sheet of about 1.6 g, 1.4 mm thickness and 10 cm^2 in area was excised from rats weighing 250–430 g.

Estimated Error:
See standard deviation in Table above.

References:
[1]T. Kawashiro, A. Campos Carles, S. F. Perry, and J. Piiper, Pflugers Arch. **359**, 219 (1975).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Dog blood and lung tissue.

Original Measurements:
I. H. Young and P. D. Wagner, J. Appl. Physiology **46**, 1207–1210 (1979).

Variables:
T/K = 310.15

Prepared By:
C. L. Young

Experimental Values

T/K	Component 2	Solubility $S \pm$ S.D.	Number of Observations	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]
310.15	Dog blood	0.00129 ± 0.00016	18	0.0863
310.15	Dog lung tissue	0.00472 ± 0.0010	25	0.0316

The solubility, $S = 10^2$ (Volume of gas dissolved converted to 1 atm pressure) Volume of liquid × 760.

The compiler calculated the Bunsen coefficient, assuming Henry's law behavior up to 1 atm pressure.

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 10 cm^3 of each sample was introduced into a 50 cm^3 syringe with 30 cm^3 of a gas mixture containing 0.0011 mole % of sulfur hexafluoride. After equilibration the gas phase was analyzed by gas chromatography. All gas was expelled from the syringe and 15 cm^3 of nitrogen gas was added and requilibrated. Samples of the gas were analyzed by gas chromatography. Details are in the source.

Source and Purity of Material:
(1) Nothing specified.
(2) The lung tissue was obtained from eight mongrel dogs. Each animal being heparinized before being killed. Lung tissue allowed to drain and then portions with few major vessels and cartilage homogenized. The blood was obtained from some of the animals.

Estimated Error:
δT/K = ±0.1
See also standard deviations above.

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Rabbit brain and blood, and saline solution.

Original Measurements:
Y. Ohta, A. Ar, and L. E. Farhi, J. Appl. Physiology **6**, 1169–1170 (1979).

Variables:
T/K = 310.15

Prepared By:
C. L. Young

Experimental Values

t/K	Component 2	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]	Number of Animals
310.15	Rabbit Blood Heparinized	0.00718 ± 0.00025	5
310.15	Rabbit Brain Homogneized	0.01455 ± 0.00023	5

The partial pressure of sulfur hexafluoride was not given but was considerably less than 1 atm.

Auxiliary Information

Method/Apparatus/Procedure:
Saline, heparinized rabbit blood, and homogenized rabbit brain tissue were saturated by passing humidified gas through three vessels in series. Samples of each of the three were analyzed by GC using helium carrier gas, a molecular sieve column, and a thermal conductivity detector.
The blood sample was heparinized.
The brain was prepared by manually squeezing out blood from the brain of a freshly killed rabbit. Volume of the brain determined by saline displacement. The tissue was homogenized and diluted with an equal volume 5% low foam detergent.

Source and Purity of Material:
(1) Sulfur hexafluoride. Nothing specified.
(2) Rabbit brain and blood. See under method.

Estimated Error:
δT/K = ±0.1

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Human plasma

Original Measurements:
M. P. Hlastala, M. Meyer, G. Riepl, and P. Scheid, Undersea Biomed. Res. **7**, 297–304 (1980).

Variables:
T/K = 310.2

Prepared By:
C. L. Young

Experimental Values

Solubility of SF_6 in human plasma at 37 °C (310.2 K)

Subject I.D.	Hemocrit	Hemoglobin	Total Proteins (10^{-2} g cm^{-3})	Total Lipids (10^{-2} g cm^{-3})	Bunsen Coefficient [α/cm^{-3}(STP)cm^{-3} atm^{-1}]	Standard Error on Mean
M.H.	47	15.6	8.3	821	0.00441	0.00026
F.S.G.	40	13.6	8.1	644	0.00481	0.00055
G.H.	44	13.9	6.9	649	0.00505	0.00009
G.M.	47	16.4	7.3	640	0.00439	0.00026
T.S.	46	16.3	7.0	1240	0.00439	0.00046
C.H.	40	15.1	7.2	670	0.00478	0.0002
Mean	44.0	15.2	7.5	777	0.00494	
SEM	1.3	0.5	0.2	97	0.00027	

SEM—Standard error of the mean. The number of determinations per subject = 5 or 6.

Auxiliary Information

Method/Apparatus/Procedure:
Aliquots were equilibrated for 60 min in a rotating tonometer with a humidified gas mixture of 70% SF_6 and 30% Ar. Samples were withdrawn in a gas-tight syringe and injected into a glass vessel. The partial pressure and gas phase composition were estimated using a mass spectrometer. Bunsen coefficients were calculated assuming Henry's law and ideal gas law obeyed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Nothing specified.
(2) Human plasma. Samples obtained from six healthy nonsmoking subjects by venipuncture. Heparinized. The heparinized blood centrifuged at 13 000 rpm for 10 min.

Estimated Error:
δT/K = ±0.1 (estimated by compiler).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Human blood

Original Measurements:
M. P. Hlastala, M. Meyer, G. Riepl, and P. Scheid, Undersea Biomed. Res. **7**, 297–304 (1980).

Variables:
T/K = 310.2

Prepared By:
C. L. Young

Experimental Values

Solubility of SF_6 in human blood at 37 °C (310.2 K)

Subject I.D.	Hemocrit	Hemoglobin	Total Proteins (10^{-2} g cm^{-3})	Total Lipids (10^{-2} g cm^{-3})	Bunsen Coefficient [α/cm^{-3}(STP)cm^{-3} atm^{-1}]	Standard Error on Mean
M.H.	47	15.6	8.3	821	0.00591	0.00032
F.S.G.	40	13.6	8.1	644	0.00555	0.00033
G.H.	44	13.9	6.9	649	0.00664	0.00040
G.M.	47	16.4	7.3	640	0.00569	0.00035
T.S.	46	16.3	7.0	1240	0.00649	0.00030
C.H.	40	15.1	7.2	670	0.00649	0.00047
Mean	44.0	15.2	7.5	777	0.00600	
SEM	1.3	0.5	0.2	97	0.00019	

SEM—Standard error of the mean. The number of determinations per subject = 5 or 6.

Auxiliary Information

Method/Apparatus/Procedure:
Aliquots were equilibrated for 60 min in a rotating tonometer with a humidified gas mixture of 70% SF_6 and 30% Ar. Samples were withdrawn in a gas-tight syringe and injected into a glass vessel. The partial pressure and gas phase composition were estimated using a mass spectrometer. Bunsen coefficients were calculated assuming Henry's law and ideal gas law obeyed.

Source and Purity of Material:
(1) Sulfur hexafluoride. Nothing specified.
(2) Human blood. Samples obtained from six healthy nonsmoking subjects by venipuncture. Heparinized.

Estimated Error:
δT/K = ±0.1 (estimated by compiler).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-64-2]
(2) Rat blood and components
(2) Human blood
(2) Olive oil

Original Measurements:
R. Guitart, Revista Espanola de Fisiologia **49**, 195–202 (1993).

Variables:
T/K = 310.2

Prepared By:
H. L. Clever

Experimental Values

Solvent	t/°C	T/K	Partition Coefficient	Standard Deviation	No. of Determinations
Rat Plasma	37	310.2	0.0039	0.0004	4
Rat Blood	37	310.2	0.0076	0.0008	3
Rat blood with Heparin	37	310.2	0.0072	0.0006	10
Human Orina	37	310.2	0.0026	0.0003	6
Human Blood	37	310.2	0.0051	0.0007	3
Human Blood with Heparin	37	310.2	0.0050	0.0002	10
Olive Oil	37	310.2	0.268	0.023	9

Blood with heparin is 1.00 mL blood with 0.23 mL saline heparin.

Auxiliary Information

Method/Apparatus/Procedure:
The liquid/gas partition coefficients were obtained by a static headspace-gas chromatograph method.[1]

Source and Purity of Material:
(1) Sulfur hexafluoride. Gas chromatography gave a purity of better than 99% purity.
(2) Nothing specified.

Estimated Error:
See standard deviations in Table above.

References:
[1]R. Guitart, A. Puigdemont, and M. Arboix, J. Chromatography **491**, 271–280 (1989).

Components:
(1) Sulfur fluoride or sulfur hexafluoride; SF_6 ; [2551-62-4]
(2) Olive oil

Original Measurements:
G. G. Power and H. Stegall, J. Appl. Physiology **29**, 145–149 (1970)

Variables:
T/K = 310.15

Prepared By:
C. L. Young

Experimental Values

T/K	Bunsen Coefficient $[\alpha/cm^3(STP)cm^{-3}\ atm^{-1}]$	Number of Determinations	Standard Deviation
310.15	0.230	4	0.001

Auxiliary Information

Procedure/Apparatus/Method:
Liquid saturated with gas in a stirred cell. 5.0 cm^3 samples of gas saturated liquid removed in a calibrated syringe and amount of gas extracted by two extractions in a Van Slyke apparatus determined. Details in source and Ref. [1].

Source and Purity of Materials:
(1) Sulfur hexafluoride. Matheson Co. Sample purity 98 mole % or better.
(2) Olive oil. Nothing specified.

Error Estimate:
δT/K = ±0.1

References:
[1]G. G. Power, J. Appl. Physiology **24**, 468 (1968).

3.5. Tetrafluoromethane

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Water; H_2O; [7732-18-5]

Evaluators:
Rubin Battino, Wright State University, Dayton, OH 45435.
H. Lawrence Clever, Emory University, Atlanta, GA 30322.
May 2003

Evaluation

An evaluation of the solubility of tetrafluoromethane in water at a partial pressure of 0.101325 MPa over the temperature interval of 278.15–318.15 K.

The solubility of tetrafluoromethane is reported in 11 papers. The first paper reports qualitative observations. It is of historical interest and was not used further. The other ten papers report a total of 35 experimental values. They were fitted to a nonlinear regression of the three and four constant Clarke, Glew, and Weiss (CGW) and the Benson and Krause (BK) equations. The three constant CGW equation was chosen to represent the data. Listed below are the total number of experimental values and the number used in the final nonlinear regression.

Reference Number	Total Number of Experimental values	Number of Experimental Values used in the Final Nonlinear Regression
1	–	Qualitative, not used
2	1	0
3	5	1
4	11	11
5	6	6
6	3	3
7	2	2
8	1	1
9	1	1
10	4	3
11	1	1

The three constant CGW equation is:

$$\ln x_1 = -(117.0233 \pm 5.3019) + (158.4980 \pm 7.5349) + (47.0324 \pm 2.5384)\ln(T/100\ \mathrm{K})$$

where x_1 is the mole fraction solubility at a partial pressure of 0.101325 MPa (1 atm) and (T/100 K) the Kelvin temperature divided by 100. For the equation, $r^2 = 0.9978$ and the standard error of estimate is 0.0129. The equation predicts a minimum at 337 K.

The three constant BK equation is:

$$\ln x_1 = (4.9224 \pm 1.2717) + (12\,187.6963 \pm 748.4287)/(T/100\ \mathrm{K}) + (2\,086\,515.2081 \pm)\ln(T/100\ \mathrm{K}).$$

where the variables are as the equation above and $r^2 = 0.9979$ and the standard error of estimate is 0.0127.

Smoothed recommended mole fraction solubility values at a partial pressure of 0.101325 MPa are given at five degree intervals from 273.15 to 323.15 K in Table 9 on the following page. Ostwald coefficients and thermodynamic changes of enthalpy, entropy, and heat capacity for the solution process are also given. The values are based on the CGW equation above.

References

[1]H. Moissan, C. R. Hebd. Seances Acad. Sci. **110**, 951 954 (1890).
[2]H. M. Parmlee, Refrig. Eng. **61**, 1341–1345 (1953).
[3]T. J. Morrison and N. B. Johnstone, J. Chem. Soc. 3441–3446 (1954).
[4]J. T. Ashton, R. A. Dawe, K. W. Miller, E. B. Smith, and B. J. Stickings, J. Chem. Soc. (A) 1793–1796 (1968).
[5]W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–245 (1979).
[6]B. A. Cosgrove and J. Walkley, J. Chromatogr. **216**, 161–167 (1981).
[7]R. A. Smith, E. G. Porter, and K. W. Miller, Biochem. Biophys. Acta **645**, 327–338 (1981).
[8]T. Park, T. R. Rettich, R. Battino, D. Peterson, and E. Wilhelm, J. Chem. Eng. Data **27**, 324–326 (1982)
[9]W. Prapaitrakul and A. D. King Jr., J. Colloid Interface Sci. **106**, 186–193 (1985).
[10]P. Scharlin and R. Battino, J. Solution Chem. **21**, 67–91 (1992).
[11]A. M. Mainer, Dissertation, University of Zaragoza, Spain, 2000.

TABLE 9. Smoothed recommended values of the mole fraction solubility of tetrafluoromethane in water at a partial pressure of 0.101325 MPa, Ostwald coefficient and thermodynamic changes on solution are given at five degree intervals from 273.15 to 323.15 K

T/K	$10^6 x_1$	Ostwald Coefficient ($10^2 L/\mathrm{cm}^3\ \mathrm{cm}^{-3}$)	Enthalpy Change ($\Delta_{\mathrm{sln}}H^{\mathrm{o}}$/kJ mol^{-1})	Entropy Change ($\Delta_{\mathrm{sln}}S^{\mathrm{o}}$/J K^{-1} mol^{-1})	Heat Capacity Change ($\Delta_{\mathrm{sln}}C_p^{\mathrm{o}}$/J K^{-1} mol^{-1})
273.15	7.995	0.994_5	−24.99	−189.0	391
278.15	6.612	0.837_5	−23.01	−181.9	391
283.15	5.588	0.720_5	−21.06	−174.9	391
288.15	4.819	0.632_0	−19.10	−168.1	391
293.15	4.235	0.564_5	−17.15	−161.3	391
298.15	3.789	0.513_0	−15.19	−154.7	391
303.15	3.447	0.474_0	−13.24	−148.2	391
303.15	3.185	0.444_5	−11.28	−141.8	391
313.15	2.987	0.422_5	−9.325	−135.5	391
318.15	2.840	0.422_5	−7.370	−129.3	391
323.15	2.736	0.398_0	−5.415	−123.3	391

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Solvents:
- Ethanol; C_2H_5OH; [64-17-5]
- Diethyl ether; $C_4H_{10}O$; [60-29-7]
- Tetrachloromethane; CCl_4; [56-23-5]
- Benzene; C_6H_6; [71-43-2]
- Carbon disulfide; CS_2; [75-15-0]
- Water; H_2O; [7732-18-5]
- Sulfuric acid; H_2SO_4; [7664-93-9]
- Aq. Potassium hydroxide; KOH; [1310-58-3]
- Aq. Barium hydroxide; $Ba(OH)_2$; [17194-00-2]

Original Measurements:
H. Moissan, C. R. Hebd. Seances Acad. Sci. **110**, 951–954 (1890).

Variables:
Room temperature.

Prepared By:
H. L. Clever

Experimental Values

Qualitative observations on the solubility of CF_4 in various solvents

Solvent	Observations
Ethanol	Very soluble
Diethyl ether	Soluble
Tetrachloromethane	Soluble
Benzene	Soluble
Carbon disulfide	Slightly soluble
Water	Slightly soluble
Sulfuric acid	Slightly soluble
Aq. Potassium hydroxide	Slightly soluble
Aq. Barium hydroxide	Slightly soluble

Auxiliary Information

Method/Apparatus/Procedure:
No details given. Included for historical interest.

Source and Purity of Materials:
(1) Tetrafluoromethane. The author points out four ways to prepare CF_4. (*i*) F_2+C (very pure C), (*ii*) F_2+CCl_4, (*iii*) F_2+CH_4, (*iv*) $AgF+CCl_4$. The author used the last method. He used care to see CCl_4 and higher CF compounds were removed from the product.
(2) Various solvents. Nothing specified.

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. M. Parmelee, Refrig. Eng. **61**, 1341–1345 (1953).

Variables:
T/K = 298.2, 323.2, and 348.2
p_1 /kPa = 101.3–827

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in water at 298.2 K at 101.3, 344.6, and 689.1 kPa

t/°C	T/K	p_1 /psia	p_1 /kPa	Solubility (s_1 /lb gal^{-1})	Solubility (c_1 /mol L^{-1})	Solubility 10^5x_1
77	298.2	14.7	101.3	0.0002	0.0003	0.5
77	298.2	50	344.6	0.0005	0.0007	1.2
77	298.2	100	689.1	0.0010	0.0014	2.5

The compiler estimated the concentration and mole fraction solubility values assuming an ideal gas and Henry's law behavior.

Only the above values were tabulated. Other values were shown graphically in Figs. 3 and 9 of the original paper. Isotherms at 77 °F, 122 °F, and 167 °F were shown at pressures up to 120 psia (pounds per square inch absolute).

The author gave the following empirical equation for use over the 77 °F–167 °F temperature interval at pressures up to 120 psia.

$$\lg(K/\text{lb gal}^{-1}\ \text{psia}^{-1}) = 657.0/(t/°\text{F} - 631.4) - 3.845$$

Distribution Coeff

Note that the constant 2.845 *in the original paper is in error. It should be* 3.845.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus consisted of two parts. The first part a steel saturating cylinder for saturations above 1 atm, the second part a conical glass flask, buret, and manometer system.
Gas and water were contacted in the steel cylinder. They were stirred vigorously for 5 h. The line was purged and a saturated sample was transferred to the evacuated conical flask and buret and manometer system for measurement of the gas volume and the water weight.
At atmospheric pressure the water was saturated directly in the low pressure side of the system.

Source and Purity of Materials:
(1) Tetrafluoromethane or Freon-14. DuPont Co. product.
(2) Water. Distilled.

Estimated Error:
δt/°F = ±0.2
$\delta s_1/s_1$ = ±0.10
Gas volumes measured to ±0.1 mL.
Water weighed to ±0.1 g.

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and N. B. B. Johnstone, J. Chem. Soc. **1954**, 3441–3446.

Variables:
T/K = 279.9–311.7
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in water at 279.9–311.7 K and a partial pressure of 101.0325 kPa (1 atm)

t/°C	T/K	$10^5 x_1$	Kuenen Coefficient [10^3 S/cm^3 (STP) g^{-1} atm^{-1}]
6.7	279.9	0.52	6.5
13.1	286.3	0.45	5.6
19.0	292.2	0.40	5.6
24.7	297.9	0.40	4.5
38.5	311.7	0.30	3.7

The authors reported the solubility as cm^3 (STP) kg^{-1} at 760 mmHg. The Compiler gave the Kuenen coefficient multiplied by 10^3 which has the same numerical value. The Compiler calculated the mole fraction assuming ideal gas behavior.

Auxiliary Information

Method/Apparatus/Procedure:
The degassed water flows in a thin film down a glass absorption helix containing the gas and water vapor at a total pressure on 1 atm. The volume of gas absorbed is measured in an attached buret system. The solvent is also measured.[1]

Source and Purity of Materials:
(1) Tetrafluoromethane. Imperial Chemical Industries, Ltd. "Arcton O."
(2) Water. Nothing specified.

Estimated Error:
$\delta S/S = \pm 0.02$ (authors).

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. **1948**, 2033.

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. T. Ashton, R. A. Dawe, K. W. Miller, E. B. Smith and B. J. Stickings, J. Chem. Soc. **1968**, 1793–1796.

Variables:
T/K = 275.55–323.15
p_1 /kPa = 80–160

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in water at 275.55–323.15 K and a partial pressure of 101.325 kPa (1 atm)

t/°C	T/K	$10^6 x_1$	Kuenen Coefficient [10^3 S/cm^3 (STP) g^{-1} atm^{-1}]
2.4	275.55	7.23	9.00
5.0	278.15	6.64	8.26
10.0	283.15	5.63	7.00
15.0	288.15	4.77	5.94
20.0	293.15	4.26	5.30
25.0	298.15	3.81	4.74
30.0	303.15	3.46	4.30
35.0	308.15	3.17	3.95
40.0	313.15	3.01	3.75
45.0	318.15	2.83	3.52
50.0	323.15	2.72	3.39

The compiler calculated the mole fraction solubility values assuming an ideal gas molar volume at 273.15 K and 1 atm of 22 414 cm^3 mol^{-1}.

The authors used the smoothing equation for mol fraction:

$$\lg x_1 = 6648.32(T/\mathrm{K}) + 45.2067 \lg(T/\mathrm{K}) - 139.5793.$$

Note that the equations for CF_4 and SF_6 are reversed in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is designed to measure gas solubilities of the order of 10^{-6} mole fraction under "dry" conditions.[1] The apparatus consists of a gas buret, a 1200 cm^3 cylindrical solution vessel with magnetically driven stirrers at top and bottom and a secondary buret that also acts as a manometer. The parts are connected by 1 mm capillary tubing.
The water is degassed by boiling under vacuum for 5 h. The apparatus is evacuated and then filled. The gas and water are in contact, and the system is stirred for 12 h. Measurements are made at pressures between 600 and 1200 mmHg (80 and 160 kPa) Henry's law is obeyed. The solubility at 1 atm (101.3 kPa) is obtained by interpolation.

Source and Purity of Materials:
(1) Tetrafluoromethane. Imperial Smelting Co. Redistilled in the apparatus. Mass Spec. Anal. showed a purity of 99.9%.
(2) Water. Double distilled.

Estimated Error:
δT/K = ± 0.02 for apparatus;
= ± 0.05 for buret system (precision).
$\delta S/S = \pm 0.01$ (random); ± 0.003 (repeat).

References:
[1]J. Horiuti, Sci. Papers Inst. Phys. Chem. Res. Tokyo, **17**, 125 (1931).

Components:
(1) Tetrafluoromethane or Freon-14; CF_4; [75-73-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. Park, T. R. Rettich, R. Battino, D. Peterson, and E. Wilhelm, J. Chem. Eng. Data, **27**, 324–326 (1982).

Variables:
T/K = 298.15
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of CF_4 in water at 298.15 K and 101.325 kPa

T/K	No. of Detn's.	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Std. Dev.
298.15	5	0.004751	2.1

The Bunsen coefficient was measured on the modified apparatus 1 (see **Method** below).

The standard deviation is given as per cent standard deviation, $100\sigma/\alpha$.

Auxiliary Information

Method/Apparatus/Procedure:
Two different versions of the Scholander[1] microgasometric apparatus were used. They were housed in an air thermostat. Apparatus 1 was the modified form described by Douglas[2] and by others.
Apparatus 2 was modified by the authors. The design includes a more efficient method of degassing and transferring water to the apparatus. The apparatus itself had a 4 cm^3 compensation chamber, a 10 cm^3 equilibration chamber, and an 8 cm side arm.

Source and Purity of Materials:
(1) Freon-14. Air Products Co. Stated to be 99.7 mol % minimum purity.
(2) Water. House distilled (reverse osmosis), passed through an ion exchange column until specific resistance was 5×10^6 Ω cm.

Estimated Error:
δT/K = ±0.05
Solubility. See percent standard deviation above.

References:
[1]P. F. Scholander, J. Biol. Chem. **167**, 235 (1947).
[2]E. Douglas, J. Phys. Chem. **68**, 169 (1964).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–246 (1979).

Variables:
T/K = 278.15–303.15
p_{tot} /MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in water from 278.15 K to 303.15 K at 0.1013 MPa

t/°C	T/K	$10^6 x_1$	Std. Dev. $10^6\sigma$	Ostwald Coefficient ($10^3 L$/mL mL^{-1})	Std. Dev. $10^3\sigma$	No. of Detns.
5	278.15	6.68	0.06	8.42	0.08	6
10	283.15	5.62	0.04	7.23	0.05	3
15	288.15	4.77	0.03	6.23	0.04	3
20	293.15	4.16	0.03	5.52	0.04	3
25	298.15	3.74	0.01	5.04	0.01	4
30	303.15	3.37	0.02	4.62	0.03	5

The authors fitted their data to equations in mole fraction and the Ostwald coefficient.

$$R \ln[x_1/(p_1/\text{MPa})] = -644.701 + 30657.3/(T/\text{K}) + 90.7526 \ln(T/\text{K}) \quad (\sigma = 0.46\%)$$

$$R \ln(L/\text{mL mL}^{-1}) = -768.677 + 36293.2/(T/\text{K}) + 111.704 \ln(T/\text{K}) \quad (\sigma = 0.35\%)$$

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and procedure were similar to that described by Ben-Naim and Baer[1] as modified by Wen and Hung.[2] It consists of a mercury manometer, a gas-volume measuring buret, a dissolution cell of 2.1 or 2.4 L and a mercury reservoir. The apparatus is immersed in a water thermostat. Degassing is done with a Battino *et al.*[3] type apparatus. The cell containing the solvent is degassed, the system filled with solvent saturated gas to 1 atm total pressure. The solvent is stirred, as the gas dissolves the pressure is maintained at 1 atm until equilibrium is reached.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Gas Products. Minimum purity of 99.7% was confirmed by GLC. Used as received.
(2) Water. Distilled then passed through Milli-Q system.

Estimated Error:
δT/K = ±0.005
δp/Torr = ±3
$\delta L/L$ = ±0.0064 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]W.-Y. Wen and J. H. Hung, J. Phys. Chem. **74**, 170 (1970).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 896 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. T. Ashton, R. A. Dawe, K. W. Miller, E. B. Smith, and B. J. Stickings, J. Chem. Soc. (A), 1793–1796 (1968).

Variables:
T/K = 275.6–323.2
p_1 /kPa = 80–160

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in water at 101.3 kPa (1 atm)

t/°C	T/K	$10^6 x_1$	Kuenen Coefficient, (10^3S/cm^3 g^{-1}atm^{-1})
2.4	275.6	7.23	9.00
5.0	278.2	6.64	8.26
10.0	283.2	5.63	7.00
15.0	288.2	4.77	5.94
20.0	293.2	4.26	5.30
25.0	298.2	3.81	4.74
30.0	303.2	3.46	4.30
35.0	308.2	3.17	3.95
40.0	313.2	3.01	3.75
45.0	318.2	3.01	3.52
50.0	323.2	2.72	3.39

The compiler calculated the mole fraction solubilities assuming the ideal gas volume of 22 414 cm^3 mol^{-1}. The authors used the smoothing equation for the mole fractions:

$$\log x_1 = 6648.32/(T/\mathrm{K}) + 45.2067 \log(T/\mathrm{K}) - 139.5793$$

Note that the equations for CF_4 and SF_6 are reversed in the paper.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is designed for the measurement of gas solubilities of the order of 10^{-6} mole fraction. It allows the bulk of the gas measurements to be performed under "dry" conditions.[1] The apparatus consists of a gas buret, a 1200 cm^3 cylindrical solution vessel with magnetically driven stirrers at the top and the bottom, and a secondary buret which also acts as a manometer. The parts are connected by 1 mm capillary tubing.
The water is degassed by boiling under vacuum for 5 h. The apparatus is evacuated and then filled. The gas and water are contacted, and the system is stirred for 12 h. Measurements are made at pressures between 600 and 1200 mmHg (80–160 kPa). Henry's law is obeyed. The solubilities at 1 atm (101.3 kPa) is obtained by interpolation.

Source and Purity of Material:
(1) Tetrafluoromethane. Imperial Smelting Co. Redistilled in the apparatus. Mass Spectrometry showed a purity of 99.9%.
(2) Water. Double distilled.

Estimated Error:
δT/K = ±0.02 apparatus; ±0.05 buret (precision).
$\delta S/S$ = ±0.01 (random); ±0.003 (repeat).

References:
[1]J. Horiuti, Sci. Papers Inst. Phys. Chem. Res. Tokyo, **17**, 125 (1931).

Components:
(1) Tetrafluoromethane; (carbon tetrafluoride); (Freon 14); CF_4; [75-73-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. Scharlin and R. Battino, J. Solution Chem. **21**, 67–91 (1992).

Variables:
T/K = 288.15–318.20
p_1 /kPa = 101.325

Prepared By:
Pirketta Scharlin

Experimental Values

Ostwald coefficient and mole fraction of tetrafluoromethane dissolved in water at 288–318 K and partial pressure of 101.325 kPa

T/K	$10^2 L$ [a,b]	$10^5 x_1$ [c,b]	$10^5 x_1$ [d]
288.15	---	---	0.4874
288.19	0.6399	0.4880	0.4868
298.15	---	---	0.3802
298.17	0.5083	0.3769	0.3800
308.15	0.4592	0.3303	0.3276
318.15	---	---	0.3081

[a]L = Ostwald coefficient [cm^3 cm^{-3}].
[b]Experimental value.
[c]x_1 = mole fraction of tetrafluoromethane (corrected for nonideality).
[d]Smoothed value; calculated from the smoothing equation below

$$\ln x_1 = -178.693 + 245.958(T/100\ \mathrm{K}) + 76.6351 \ln(T/100\ \mathrm{K}).$$

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus was based on a design of Ben-Naim and Baer,[1] which had been improved by modifications described in detail in Tominaga *et al.*[2] After degassing,[3] the solvent was transferred under its own vapor pressure into the evacuated mixing chamber. The gas buret was evacuated and the system filled with the solvent-saturated gas to a total pressure of about 1 atm. The computer program controlling the apparatus read the pressure of the system, which was tracked during the measurement. When the reading was stable, the pressure was adjusted to 1 atm and the corresponding pressure transducer reading became the setpoint for pressure control. After pre-equilibration, the initial volume of solvent was determined using a precision cathetometer. The dissolution was initiated by high-speed stirring of the solvent. After the system had reached equilibrium, stirring was stopped and the final volume of solvent was recorded. Gas volume was determined by a computer counting the number of steps a stepping motor used to drive a close-fitting stainless steel or teflon piston with two O-ring seals through a Fisher and Porter precision bore tube.

Source and Purity of Material:
(1) Airco, purity 99.7 mole %.
(2) Reverse osmosis "house-distilled." Further purified by continuous pumping through a series of Illco-Way research model ion exchangers and through a 1.2 μm pore size Millipore filter. Degassed.

Estimated Error:
δT/K = ±0.03
$\delta p/p$ = ±0.2%
$\delta L/L$ = ±1.0%

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Water-d_2; D_2O; [7789-20-0]

Evaluators:
Rubin Battino, Wright State University, Dayton, OH 45435.
H. Lawrence Clever, Emory University, Atlanta, GA 30322.
2002

Evaluation

An evaluation of the solubility of tetrafluoromethane in deuterium oxide at 0.101325 MPa partial pressure between 278.15 K and 318.15 K

There are three reports of the solubility of tetrafluoromethane in heavy water. On a point by point comparison the data from Ref. 1 and 2 agree to better than 3% while Ref. 3 runs about 3.5% smaller at 288.15 K and 8.5% smaller at 298.15 K. All data accord fairly well on an $\ln x_1$ vs. T/K plot and all of the data were fit to both the three constant Clark, Glew, and Weiss equation and the three constant Benson and Krause equation with equally satisfactory results. The fitted equations are:

Clark, Glew and Weiss (CGW)

$$\ln x_1 = -99.6192 + 136.6155/(T/100\ \mathrm{K}) + 37.9044 \ln(T/100\ \mathrm{K})$$

with $r^2 = 0.9919$ and standard error of estimate $\sigma = 0.0304$.

Benson and Krause (BK)

$$\ln x_1 = -1.4143 - 8892.9037/(T/\mathrm{K}) + 1\,675\,725.0310(T/\mathrm{K})^2$$

with $r^2 = 0.9918$ and standard error of estimate $\sigma = 0.0306$.

The experimental data do not extend to a high enough temperature to locate a minimum in the solubility curve. The CGW equation predicts a minimum near 360 K and the BK equation predicts the minimum at 377 K.

Below are values of tentative mole fraction solubility at a partial pressure of 0.101325 MPa, Ostwald coefficient and the thermodynamic changes on solution at five degree intervals from 278.15 K to 318.15 K as calculated from the CGW equation (see Table 10). Figure 2 shows the fitted equation and the experimental points.

References

[1]W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–245 (1979).
[2]B. A. Cosgrove and J. Walkley, J. Chromatogr. **216**, 161–167 (1981).
[3]P. Scharlin and R. Battino, J. Solution Chem. **21**, 67–91 (1992).

TABLE 10. Smoothed tentative values of the mole fraction solubility of CF_4 in D_2O at a partial pressure of 0.101325 MPa, the Ostwald coefficients and the thermodynamic changes on solution between 278.15 K and 318.15 K

T/K	$10^6 x_1$	Ostwald, Coefficient ($10^2 L/\mathrm{cm}^3\ \mathrm{cm}^{-3}$)	$\Delta_{sln}H^o{}_1$ /kJ mol^{-1}	$\Delta_{sln}S^o{}_1$ /J K^{-1} mol^{-1}	$\Delta_{sln}C_p{}^o{}_1$ /J K^{-1} mol^{-1}
278.15	8.067	1.016	−25.93	−190.7	315
283.15	6.658	0.854	−24.35	−185.1	315
288.15	5.596	0.731	−22.78	−179.6	315
293.15	4.785	0.572	−21.20	−174.2	315
298.15	4.158	0.505	−19.63	−168.8	315
303.15	3.668	0.452	−18.05	−163.6	315
308.15	3.278	0.411	−16.47	−158.4	315
313.15	2.977	0.379	−14.90	−153.4	315
318.15	2.734	0.353	−13.32	−148.4	315

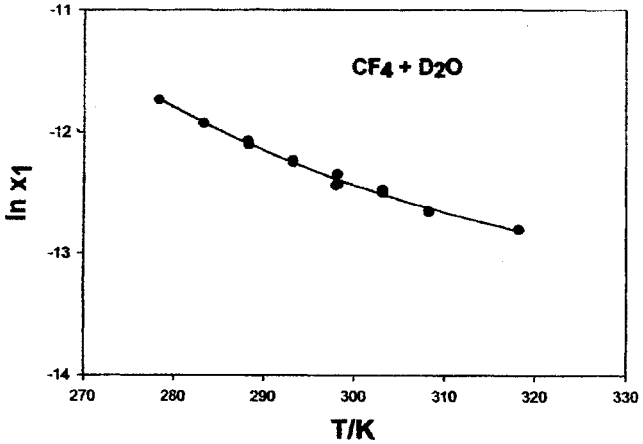

FIG. 2. Tetrafluoromethane+deuterium oxide: $\ln x_1$ vs T/K. Fitted equation and 13 experimental values.

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Water-d_2 ; D_2O; [7789-20-0]

Original Measurements:
W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–246 (1979).

Variables:
T/K = 278.15–303.15
p_{tot} /MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in water-d_2 from 278.15 K to 303.15 K at 0.1013 MPa

t/°C	T/K	$10^6 x_1$	Std. Dev. $10^6\sigma$	Ostwald Coefficient ($10^3 L$/mL mL^{-1})	Std. Dev. $10^3\sigma$	No. of Det'n.
5	278.15	8.02	---	10.05	---	1
10	283.15	6.62	---	8.45	---	1
15	288.15	5.74	0.02	7.46	0.02	2
20	293.15	4.79	---	6.37	---	1
25	298.15	4.36	---	5.85	---	1
25	303.15	3.83	0.07	5.22	0.09	2

The authors fitted their data to equations in mole fraction and the Ostwald coefficient.

$$R \ln[x_1/(p_1/\text{MPa})] = -437.270 + 22\,133.4/(T/\text{K}) + 59.4112 \ln(T/\text{K}) \quad (\sigma = 0.76\%]$$

$$R \ln(L/\text{mL mL}^{-1}) = -811.846 + 38\,654.5/(T/\text{K}) + 117.933 \ln(T/\text{K}) \quad (\sigma = 0.35\%)$$

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and procedure were similar to that described by Ben-Naim and Baer[1] as modified by Wen and Hung.[2] It consists of a mercury manometer, a gas-volume measuring buret, a dissolution cell of 2.1 or 2.4 L and a mercury reservoir. The apparatus is immersed in a water thermostat. Degassing is done with a Battino *et al.*[3] type apparatus. The cell containing the solvent is degassed, the system filled with solvent saturated gas to 1 atm total pressure. The solvent is stirred, as the gas dissolves the pressure is maintained at 1 atm until equilibrium is reached.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Gas Products. Minimum purity of 99.7% was confirmed by GLC. Used as received.
(2) Water-d_2 . Stohler Isotope Chemicals Co. Specified to be 99.8%. Used as received.

Estimated Error:
δT/K = ±0.005
δp/Torr = ±3
$\delta L/L$ = ±0.0064 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]W.-Y. Wen and J. H. Hung, J. Phys. Chem. **74**, 170 (1970).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 896 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Water; H_2O; [7732-18-5]
(2) Water-d_2 ; D_2O; [7789-20-0]

Original Measurements:
B. A. Cosgrove and J. Walkley, J. Chromatogr. **216**, 161–167 (1981).

Variables:
T/K = 293.15, 298.15, and 303.15
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of CF_4 in water, H_2O

T/K	$10^4 x_1$
293.15	0.04174
298.15	0.03750
303.15	0.03492

Solubility of CF_4 in water-d_2 , D_2O.

T/K	$10^4 x_1$
293.15	0.04174
303.15	0.03719

Auxiliary Information

Method/Apparatus/Procedure:
A 20 mL volume of degassed solvent (sublimation technique) is transferred to a previously evacuated (10^{-4} mmHg) saturation cell immersed in an insulated controlled (±0.01 K) water thermostat. The gas is dispersed through the constantly stirred solution at 1 atm by a coarse fritted glass disc. Saturation is obtained within a few hours. Prior to analysis the solution is allowed to sit under I am gas pressure for 1 h. A saturated sample is withdrawn from the saturation cell using a greaseless, gas tight (2.500±0.001 mL) Gilmont syringe. A 0.250 mL portion is injected "wet" the frit. It is stripped and then four 0.500 mL samples are injected sequentially into the cell. The stripped gas is dried before entering the column. The gas is analyzed on a dual filament conductivity detector. Calibrations are made with pure gas dry before and wet after each series of runs.

Source and Purity of Material:
(1) Tetrafluoromethane. Nothing specified.
(2) Water. Nothing specified.
(2) Water-d_2 . Nothing specified.

Estimated Error:
δt/K = ±0.01
$\delta x_1/x_1$ = ±0.15

Components:
(1) Tetrafluoromethane; (carbon tetrafluoride); (Freon 14); CF_4; [75-73-0]
(2) Water-d_2; (deuterium oxide); D_2O; [7789-20-0]

Original Measurements:
P. Scharlin and R. Battino, J. Solution Chem. **21**, 67–91 (1992).

Variables:
T/K = 288.15–318.23
p_1 /kPa = 101.325

Prepared By:
Pirketta Scharlin

Experimental Values

Ostwald coefficient and mole fraction of tetrafluoromethane dissolved in deuterium oxide at 288–318 K and partial pressure of 101.325 kPa

T/K	10^2L [a,b]	10^5x_1 [c,b]	10^5x_1 [d]
288.15	—	—	0.5540
288.21	0.7193	0.5532	0.5527
297.97	0.5337	0.3971	0.4010
298.15	—	—	0.3990
298.17	0.5381	0.4004	0.3988
308.15	—	—	0.3174
308.16	0.4444	0.3207	0.3174
308.18	0.4402	0.3176	0.3173
318.15	—	—	0.2757
318.18	0.3924	0.2752	0.2756
318.23	0.3926	0.2753	0.2755

[a] L = Ostwald coefficient [$cm^3\ cm^{-3}$].
[b] Experimental value.
[c] x_1 = mole fraction of tetrafluoromethane (corrected for nonideality).
[d] Smoothed value; calculated from the smoothing equation below $\ln x_1 = -171.010 + 238.782/(T/100\ \mathrm{K}) + 71.8496 \ln(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus was based on a design of Ben-Naim and Baer[1] which had been improved by modifications described in detail in Tominaga *et al.*[2] After degassing,[3] the solvent was transferred under its own vapor pressure into the evacuated mixing chamber. The gas buret was evacuated and the system filled with the solvent-saturated gas to a total pressure of about 1 atm. The computer program controlling the apparatus read the pressure of the system which was tracked during the measurement. When the reading was stable, the pressure was adjusted to 1 atm and the corresponding pressure transducer reading became the setpoint for pressure control. After pre-equilibration, the initial volume of solvent was determined using a precision cathetometer. The dissolution was initiated by high-speed stirring of the solvent. After the system had reached equilibrium, stirring was stopped and the final volume of solvent was recorded. Gas volume was determined by a computer counting the number of steps a stepping motor used to drive a close-fitting stainless steel or teflon piston with two O-ring seals through a Fisher and Porter precision bore tube.

Source and Purity of Material:
(1) Airco, purity 99.7 mole %.
(2) Aldrich, 99.8 mole %. Degassed.

Estimated Error:
δT/K = ±0.03
$\delta p/p$ = ±0.2%
$\delta L/L$ = ±1.0%

References:
[1] A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2] T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data, **31**, 175 (1986).
[3] R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; (carbon tetrafluoride); (Freon 14); CF_4; [75-73-0]
(2) Seawater

Original Measurements:
P. Scharlin and R. Battino, J. Chem. Eng. Data, **40**, 167–169 (1995).

Variables:
T/K = 288.15–303.15
p_1 /kPa = 101.325

Prepared By:
Pirketta Scharlin

Experimental Values

Ostwald coefficient and molality of tetrafluoromethane dissolved in water and seawater at 288–303 K and partial pressure of 101.325 kPa

T/K	S/‰ [a]	10^2L [b,c]	10^3m_1 /mol kg^{-1} [d,c]
288.15	0.000	0.6385 [e]	0.2703 [e]
288.15	35.086	0.5169	0.2130
293.15	0.000	0.5647 [e]	0.2352 [e]
293.15	35.086	0.4527	0.1836
298.15	0.000	0.5128 [e]	0.2102 [e]
298.15	35.086	0.4027	0.1608
303.15	0.000	0.4773 [e]	0.1927 [e]
303.15	35.086	0.3635	0.1430

[a] S = salinity (in Practical Salinity Scale 1978).
[b] L = Ostwald coefficient [$cm^3\ cm^{-3}$].
[c] Smoothed values; the smoothing equation for values in the seawater of salinity of 35.086‰ was $\ln L = -93.8568 + 136.046(T/100\ \mathrm{K}) + \ln(T/100\ \mathrm{K})$.
[d] m_1 = molality of tetrafluoromethane.
[e] Values in H_2O are from P. Scharlin and R. Battino, J. Solution Chem. **21**, 67–91 (1992).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus was based on a design of Ben-Naim and Baer,[1] which had been improved by modifications described in detail in Tominaga *et al.*[2] After degassing,[3] the solvent was transferred under its own vapor pressure into the evacuated mixing chamber. The gas buret was evacuated and the system filled with the solvent-saturated gas to a total pressure of about 1 atm. The computer program controlling the apparatus read the pressure of the system, which was tracked during the measurement. When the reading was stable, the pressure was adjusted to 1 atm and the corresponding pressure transducer reading became the setpoint for pressure control. After pre-equilibration, the initial volume of solvent was determined using a precision cathetometer. The dissolution was initiated by high-speed stirring of the solvent. After the system had reached equilibrium, stirring was stopped and the final volume of solvent was recorded. Gas volume was determined by a computer counting the number of steps a stepping motor used to drive a close-fitting stainless steel or teflon piston with two O-ring seals through a Fisher and Porter precision bore tube.

Source and Purity of Material:
(1) Airco, purity 99.7 mole %.
(2) Scripps Institution of Oceanography. The surface seawater was poisoned with 100 μL of saturated mercuric chloride per liter, and was allowed to evaporate approximately 3% to increase its salinity. It was filtered through a 1 μm filter, mixed in a glass carboy, and subsampled for the determination of its salinity by conductivity. The salinity was reported to be 35.086‰.

Estimated Error:
δT/K = ±0.03
$\delta p/p$ = ±0.2%
$\delta L/L$ = ±1.0%

References:
[1] A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2] T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[3] R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:

(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Water; H_2O; [7732-18-5]
(3) Electrolytes:
• *N,N,N*-Trimethyl-decanaminium bromide; $C_{13}H_{30}N.Br$; [2082-84-5]
• *N,N,N*-Trimethyl-1-hexadecanaminium bromide; $C_{19}H_{42}N.Br$; [57-09-0]
• Lithium salt Nonadecafuorodecanoic acid; $LiC_{10}F_{19}O_2$; [84743-32-8]
• Sulfuric acid monododecyl ester sodium salt; $C_{12}H_{26}O_4$. Na; [151-21-3]
• Potassium chloride; KCl; [7447-40-7]
• Sodium chloride; NaCl; [7647-14-5]

Evaluators:

H. Lawrence Clever, Emory University,
Atlanta, GA 30322-2210
2002

Evaluation

An evaluation of the solubility of tetrafluoromethane in aqueous electrolyte solutions.

Refer to the first two pages of the evaluation of sulfur hexafluoride+electrolyte+water systems earlier in this paper for general background on salt effects. There is surprisingly little data on the solubility of tetrafluoromethane in the aqueous common inorganic electrolytes. The first report was Moissan,[1] the discoverer of tetrafluoromethane, in 1890. He reported that the gas was insoluble in sulfuric acid [7664-93-9], aqueous potassium hydroxide [1310-58-3], and aqueous barium hydroxide [17194-00-2]. This is a qualitative observation and it is rejected. The other reports on salt effects are given below. Most of them report studies of micelle formation of dilute solutions of surfactants and an enhanced solubility due to the gas dissolving in the micelle to a greater extent than in water.

Tetrafluoromethane+N,N,N-Trimethyl-decanaminium bromide+Water

Prapaitrakul and King[3] measured the solubility of tetrafluoromethane at 299 K in water and six surfactant solutions from 0.04 to 0.50 mol kg^{-1}. At 0.50 mol kg^{-1} surfactant the CF_4 solubility increased 67% of its value in water. The data are classed tentative.

Tetrafluoromethane+N,N,N-Trimethyl-1-hexadecanaminium bromide+Water.

Prapaitrakul and King[3] measured the solubility of tetrafluoromethane at 299 K in water and three surfactant solutions from 0.10 to 0.30 mol kg^{-1}. At 0.30 mol kg^{-1} surfactant the CF_4 solubility increased 107% of its value in water. The data are classed tentative.

Tetrafluoromethane+Lithium salt of nonadecafuorodecanoic acid+Water

Prapaitrakul and King[4] measured the solubility of tetrafluoromethane at 299 K in water and three surfactant solutions from 0.10 to 0.30 mol kg^{-1}. At 0.30 mol kg^{-1} surfactant the CF_4 solubility increased 467% of its value in water. The data are classed tentative.

Tetrafuoromethane+Sulfuric acid monod odecyl ester sodium salt+Water

Prapaitrakul and King[3] measured the solubility of tetrafluoromethane at 299 K in water and three surfactant solutions from 0.10 to 0.50 mol kg^{-1}. At 0.50 mol kg^{-1} surfactant the CF_4 solubility increased 115% of its value in water. The data are classed tentative.

Tetrafluoromethane+Potassium chloride+Water

Smith, Porter and Miller[2] measured the Bunsen coefficient, α/cm^3 (STP) cm^{-3} atm^{-1}, of tetrafluoromethane in water and in a buffer solution containing 0.15 mol L^{-1} KCl, 0.01 mol L^{-1} tris-HCl and 0.02 mol L^{-1} $Na(N_3)$ at a partial pressure of 35 atm (3.55 MPa) at the temperatures of 284.7 and 298.2 K. The total concentration of 1-1 electrolyte was taken as 0.18 mol L^{-1}. The author calculated salt effect parameters of 0.289 and 0.320 for temperatures 284.7 and 298.2, respectively. The mixture of electrolytes and the high pressure of the experiment make it difficult to judge the usefulness of these values. The increase in salt effect parameter magnitude with temperature is contrary to most observations. The salt effect magnitude is much larger than usually observed for KCl alone.

Tetrafluoromethane+Sodium chloride+Water

Smits, Smits, Peters, and de Swaan Arons[5] describe high pressure (20–200 MPa) high temperature (580–673 K) behavior of the system. Both the CF_4+H_2O and the $CF_4+NaCl+H_2O$ systems were studied. Although not a conventional salt effect study it may be of interest to some.

References

[1]H. Moissan, C. R. Hebd. Acad. Sci. **110**, 951–954 (1890).
[2]R. A. Smith, E. G. Porter and K. W. Miller, Biochem. Biophys. Acta **645**, 327–338 (1981).
[3]W. Prapaitrakul and A. D. King, Jr., J. Colloid Interface Sci. **106**, 186–193 (1985).
[4]W. Prapaitrakul and A. D. King, Jr., J. Colloid Interface Sci. **118**, 224–232 (1987).
[5]P. J. Smits, R. J. A. Smits, C. J. Peters, and J. de Swaan Arons, J. Chem. Thermodyn. **29**, 23–30 (1997); J. Chem. Thermodyn. **29**, 385–393 (1997).

Components:

(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. J. Smits, R. J. A. Smits, C. J. Peters, and J. de Swaan Arons, J. Chem. Thermodyn. **29**, 23–30 (1997); J. Chem. Thermodyn. **29**, 385–393 (1997).

Variables:

T/K = 580–673
p/MPa = 20–200

Prepared By:

H. L. Clever

Experimental Values

These two papers describe the high pressure behavior of the systems $\{xCF_4+(1-x)H_2O\}$ and $\{x_1CF_4+x_2NaCl+(1-x_1-x_2)H_2O\}$. The data are not compiled, but the papers are noted as natural extensions of the low pressure data compiled here. A brief summary of the experiments is given.

$\{xCF_4+(1-x)H_2O\}$

(Gas+gas) equilibria for ten compositions, with $(0.0121\pm0.0002)<x<(0.0583\pm0.0002)$ were measured over the pressure range from 20 to 200 MPa and temperature range of 580–673 K. The system exhibits type-III fluid phase behavior.

$\{x_1CF_4+x_2NaCl+(1-x_1-x_2)H_2O\}$

(Gas+Gas) equilibria for ten compositions, with mole fractions of CF_4 $(0.0076\pm0.0002)<x_1<(0.0335\pm0.0002)$ and NaCl$(0.0032\pm0.0002)<x_2<(0.0103\pm0.0002)$ were measured over the pressure range from 20–200 MPa and the temperature range of 585–663 K.

The paper contains extensive data and other details.

Auxiliary Information

Method/Apparatus/Procedure:

The experiments were carried out in a high pressure autoclave with sapphire windows and magnetic stirring.

Source and Purity of Material:

(1) Tetrafluoromethane. Praxair N. V. Belgium. Minimum purity 0.99995. Used as received.
(2) Sodium chloride. Merck, Germany. Suprapur®. Minimum mass fraction purity is 0.995 guaranteed. Used as received.
(3) Water. Laboratory source. Double distilled.

Estimated Error:

Nothing specified.

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) *N,N,N*-Trimethyl-decanaminium.bromide; $C_{13}H_{30}N.Br$; [2051-84-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
W. Prapaitrakul and A. D. King, Jr., J. Colloid Interface Sci. **106**, 186–193 (1985).

Variables:
$T/K = 299$
m_2 /mol kg^{-1} = 0–0.50

Prepared By:
H. L. Clever

Experimental Values
Solubility of CF_4 in aqueous DTAB at 26 °C (299 K)

Surfactant[a] (m_2 /mol kg^{-1})	CF_4 Solubility[b] ($10^3 m_1$ /mol kg^{-1} atm^{-1})
0.0	0.27[b]
0.04	0.29
0.10	0.28
0.20	0.36
0.30	0.41
0.40	0.43
0.50	0.45

[a]Other names for component 2 are Decyltrimethyl ammonium bromide and DTAB.
[b]The solubility of CF_4 in water corresponds to a mole fraction of 4.9×10^{-6} at a partial pressure of 1 atm.

Auxiliary Information

Method/Apparatus/Procedure:
The procedure consists of three steps: (*i*) the solution is allowed to equilibrate with the gas at an elevated pressure in a thermostated bomb equipped with a magnetic stirrer; (*ii*) the stirrer is stopped and the solution allowed to become still, whereupon the pressure is released to its ambient value; (*iii*) after a short delay in order to re-establish thermal equilibrium the stirrer is activated and the gas released from the supersaturated solution is collected manometrically at ambient conditions. A series of such measurements from different saturating final pressure are made. A plot of (Δn/mol) vs (Δp/atm) is linear and the slope defines the solubility.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Stated to be >99.7%.
(2) DTAB. Eastman Kodak Co. No stated purity. Recrystallized from 2-propanol and dried *in vacuo*.
(3) Water. Double distilled.

Estimated Error:
Temperature: Nothing specified.
δm_1 /mol kg^{-1} = $\pm 0.02\times10^{-3}$ (precision, authors).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) *N,N,N*-Trimethyl-1-hexadecanaminium.bromide; $C_{19}H_{42}N.Br$; [57-09-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
W. Prapaitrakul and A. D. King, Jr., J. Colloid Interface Sci. **106**, 186–193 (1985).

Variables:
$T/K = 299$
m_2 /mol kg^{-1} = 0–0.30

Prepared By:
H. L. Clever

Experimental Values
Solubility of CF_4 in aqueous DTAB at 26 °C (299 K)

Surfactant[a] (m_2 /mol kg^{-1})	CF_4 Solubility[b] ($10^3 m_1$ /mol kg^{-1} atm^{-1})
0.0	0.27
0.10	0.42
0.20	0.42
0.30	0.56

[a]Other names for component 2 are Cetyltrimethyl ammonium bromide and CTAB.
[b]The solubility of CF_4 in water corresponds to a mole fraction of 4.9×10^{-6} at a partial pressure of 1 atm.

Auxiliary Information

Method/Apparatus/Procedure:
The procedure consists of three steps: (*i*) the solution is allowed to equilibrate with the gas at an elevated pressure in a thermostated bomb equipped with a magnetic stirrer; (*ii*) the stirrer is stopped and the solution allowed to become still, whereupon the pressure is released to its ambient value; (*iii*) after a short delay in order to re-establish thermal equilibrium the stirrer is activated and the gas released from the super-saturated solution is collected manometrically at ambient conditions. A series of such measurements from different saturating final pressure are made. A plot of (Δn/mol) vs (Δp/atm) is linear and the slope defines the solubility.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Stated to be >99.7%.
(2) CTAB. Aldrich Chem. Co. Stated purity 95%. Recrystallized from 2-propanol and dried *in vacuo*.
(3) Water. Double distilled.

Estimated Error:
Temperature: Nothing specified.
δm_1 /mol kg^{-1} = $\pm 0.02\times10^{-3}$ (precision, authors).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Sulfuric acid monododecyl ester sodium salt; $C_{12}H_{26}O_4$. Na; [151-21-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
W. Prapaitrakul and A. D. King, Jr., J. Colloid Interface Sci. **106**, 186–193 (1985).

Variables:
T/K = 299
m_2 /mol kg^{-1} = 0–0.50

Prepared By:
H. L. Clever

Experimental Values

Solubility of CF_4 in aqueous DTAB at 26 °C (299 K)

Surfactant[a] (m_2 /mol kg^{-1})	CF_4 Solubility[b] ($10^3 m_1$ /mol kg^{-1} atm^{-1})
0.0	0.27
0.10	0.37
0.30	0.48
0.50	0.58

[a]Other names for component 2 are Sodium dodecyl sulfate and SDS.
[b]The solubility of CF_4 in water corresponds to a mole fraction of 4.9×10^{-6} at a partial pressure of 1 atm.

Auxiliary Information

Method/Apparatus/Procedure:
The procedure consists of three steps: (*i*) the solution is allowed to equilibrate with the gas at an elevated pressure in a thermostated bomb equipped with a magnetic stirrer; (*ii*) the stirrer is stopped and the solution allowed to become still, whereupon the pressure is released to its ambient value; (*iii*) after a short delay in order to re-establish thermal equilibrium the stirrer is activated and the gas released from the super-saturated solution is collected manometrically at ambient conditions. A series of such measurements from different saturating final pressure are made. A plot of (Δn/mol) vs (Δp/atm) is linear and the slope defines the solubility.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Stated to be >99.7%.
(2) SDS. BDH Product No. 44244, Lot No. 9088113C. Stated purity 99%. Recrystallized from 2-propanol and dried *in vacuo*.
(3) Water. Double distilled.

Estimated Error:
Temperature: Nothing specified.
δm_1 /mol kg^{-1} = $\pm0.02\times10^{-3}$ (precision, authors).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Lithium salt of nonadecafluorodecanoic acid; $LiC_{10}F_{19}O_2$; [84743-32-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
W. Prapaitrakul and A. D. King, Jr., J. Colloid Interface Sci. **118**, 224–232 (1987).

Variables:
T/K = 299
m_2 /mol kg^{-1} = 0–0.30

Prepared By:
H. L. Clever

Experimental Values

Solubility of CF_4 in aqueous DTAB at 26 °C (299 K)

Surfactant[a] (m_2 /mol kg^{-1})	CF_4 Solubility[b] ($10^3 m_1$ /mol kg^{-1} atm^{-1})
0.0	0.27
0.10	0.79
0.20	1.19
0.30	1.53

[a]Other names for component 2 are Lithium perfluorodecanoate and LiPFD.
[b]The solubility of CF_4 in water corresponds to a mole fraction of 4.9×10^{-6} at a partial pressure of 1 atm. The water value is from W. Prapaitrakul and A. D. King, Jr., J. Colloid Interface Sci. **106**, 186 (1985).

Auxiliary Information

Method/Apparatus/Procedure:
The procedure consists of three steps: (*i*) the solution is allowed to equilibrate with the gas at an elevated pressure in a thermostated bomb equipped with a magnetic stirrer; (*ii*) the stirrer is stopped and the solution allowed to become still, whereupon the pressure is released to its ambient value; (*iii*) after a short delay in order to re-establish thermal equilibrium the stirrer is activated and the gas released from the super-saturated solution is collected manometrically at ambient conditions. A series of such measurements from different saturating final pressure are made. A plot of (Δn/mol) vs. (Δp/atm) is linear and the slope defines the solubility.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Stated to be >99.7%.
(2) Lithium perfluorodecanoate. Prepared by titration of LiOH with oerfluorodecanoic acid to pH 9–12.
(3) Water. Double distilled.

Estimated Error:
Temperature: Nothing specified.
δm_1 /mol kg^{-1} = $\pm0.01\times10^{-3}$ (precision, authors).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Water; H_2O; [7732-18-5]
(2) Aqueous Buffer containing:
- Potassium chloride; KCl; [7447-40-7]
- Sodium azide; NaN_3 ; [26628-22-8]
- Tris(hydroxymethyl)aminomethane hydrochloride (Tris-HCl); $(HOCH_2)_3CNH_2$ .HCl; [1185-53-1]

(2) Lipid biolayers+Cholesterol; [57-88-5]

Original Measurements:
R. A. Smith, E. G. Porter, and K. W. Miller, Biochem. Biophys. Acta **645**, 327–338 (1981).

Variables:
T/K=284.7, 298.2
p_1 /MPa=3.55

Prepared By:
H. L. Clever

Experimental Values

Temperature (t/°C)	Temperature T/K	Partial Pressure (p_1 /atm)	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]
		Water; H_2O; [7732-18-5] Literature[1]	
11.5	284.7	35.0	0.00665
25.0	298.2	35.0	0.00475
		Buffer [0.15 mol L^{-1} KCl], 0.1 mass % NaN_3 , 10 mmol L^{-1} Tris-HCl, pH=7.4.	
11.5	284.7	35.0	0.00590
25.0	298.2	35.0	0.00416
		Egg phosphatidylcholine, 96%, phosphatidic acid 4%	
11.5	284.7	35.0	0.0555
25.0	298.2	35.0	0.0563
		Egg phosphatidylcholine, 64%; phosphatidic acid, 3%; Cholesterol, 33% (PC/PA/Chol)	
11.5	284.7	35.0	0.0329
25.0	298.2	35.0	0.0437

Auxiliary Information

Method/Apparatus/Procedure:
Authors' apparatus II. Six 18 mL glass cuvetts, each with a Teflon coated magnetic stirring button equipped with a stainless steel wire that broke the surface, are mounted inside a 50 mm internal diameter pressure cylinder. Six stainless steel tubes, 0.26 μL (mm)$^{-1}$, passed through the disc top of the pressure vessel with one tube going to the bottom of each cuvett. The cuvetts contained either water, buffer, or one of the phospholipid suspensions. The pressure chamber was flushed with the gas under study, then sealed and pressurized with the gas. After 12 h equilibration the cuvetts were sampled in turn by slowly bleeding 0.75 mL of solution at 0.5 mL m^{-1} through a 300 μL sample loop. With a micrometer metering valve. The sample loop was decompressed and its contents flushed into a stripping device. The stripped gas went to a gas chromatograph for analysis.

Source and Purity of Material:
(1) Tetrafluoromethane. Nothing specified.
(2) Water and buffer. Nothing specified. Egg phosphatidyl choline and egg phosphtidic acid. Lipid Products. Nutfield. Cholesterol. Sigma Chemical Co. Re-crystallized from methanol. The phospholipids with or without cholesterol were dried down from $CHCl_3$ solution and suspended in the buffer by vortexing and then sonification. Centrifugation yielded translucent suspensions of 10–46 mg (mL)$^{-1}$.

Estimated Error:
δT/K=±0.1
$\delta\alpha/\alpha$=±0.035–0.050 (compiler).

References:
[1]R. K. Stoelting and R. E. Longshore, Anesthesiology **36**, 503 (1972)
[2]For more on method see: K. W. Miller, L. Hammond, and E. Porter, Chem. Phys. Lipids **20**, 229 (1977).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [77253-67-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
A. M. Mainar, Dissertation, Universidad de Zaragoza, Spain 2000.

Variables:
T/K=298.15
p_1 /kPa=101.33
x_2=0–1.0; x_3=1.0–0

Prepared By:
H. L. Clever

Experimental Values
Saturated solution properties at 298.15 K

Solvent: x_2 for $C_2H_3F_3O$	Solvent Density (ρ/g cm^{-3})	Gibbs Energy of Solution ($\Delta G°_3$ /kJ mol^{-1})	CF_4 Solubility 10^4x_1	Henry's Constant [ln(K_H /Pa)]
0	0.99707	30.92	0.0382	24.00
0.0293	1.04690	30.94	0.0380	24.00
0.0614	1.09218	29.74	0.0617	23.52
0.0997	1.13590	27.32	0.1633	22.55
0.1445	1.17653	25.40	0.3551	21.77
0.1954	1.21259	23.89	0.6523	21.16
0.2685	1.25140	23.89	1.171	20.58
0.3633	1.28717	21.07	2.036	20.02
0.4942	1.32086	19.72	3.511	19.48
0.6726	1.35073	18.23	6.402	18.88
1	1.38209	18.23	13.14	18.16

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent vapor saturated gas.

Source and Purity of Material:
(1) Carbon tetrafluoride. J. T. Baker Co. Stated to be 99 mol %.
(2) 2,2,2-Trifluoroethanol. Flurchem Ltd. Stated to be >99%.
(3) Water. Double distilled and deionized (Milli-Q).

Estimated Error:
δT=±0.05 cell, ±0.2 burets;
$\delta x_1/x_1$=±0.007 (author).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallarado, J. S. Urieta, and C. Guteirrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1,1,1,3,3,3-Hexafluoropropanol-2; C_3HF_6O; [920-66-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
A. M. Mainar, Dissertation, Universidad de Zaragoza, Spain 2000.

Variables:
T/K = 298.15
p_1 /kPa = 101.33
x_2 = 0 – 1.0; x_3 = 1.0 – 0

Prepared By:
H. L. Clever

Experimental Values

Saturated solution properties at 298.15 K

Solvent: x_2 for C_3HF_6O	Solvent Density (ρ/g cm^{-3})	Gibbs Energy of Solution ($\Delta G°_3$ /kJ mol^{-1})	CF_4 Solubility $10^4 x_1$	Henry's Constant (ln(K_H /Pa))
0	0.99707	30.92	0.0382	24.00
0.0186	1.06351	30.08	0.0538	23.66
0.0419	1.13258	27.06	0.1813	22.44
0.0682	1.19615	24.87	0.4395	21.55
0.1030	1.26294	23.27	0.8373	20.91
0.1461	1.32593	21.99	1.403	20.39
0.2008	1.38476	20.74	2.324	19.89
0.2890	1.44869	19.33	4.102	19.32
0.4116	1.50304	17.83	7.523	18.71
0.6230	1.55480	17.83	15.39	18.00
0.8154	1.58280	14.97	23.84	17.56
1	1.60423	14.23	32.16	17.26

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent vapor saturated gas.

Source and Purity of Material:
(1) Carbon tetrafluoride. J. T. Baker Co. Stated to be 99 mol %.
(2) 1,1,1,3,3,3-Hexafluoropropanol-2. Flurchem Ltd. Stated to be >99%.
(3) Water. Double distilled and deionized (Milli-Q).

Estimated Error:
$\delta T = \pm 0.05$ cell, ± 0.2 burets;
$\delta x_1 / x_1 = \pm 0.007$ (author).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979)
[2]M. A. Gallarado, J. S. Urieta, and C. Guteirrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Alkanes (C_6 to C_{16}):
Hexane; C_6H_{14} ; [110-54-3]
Heptane; C_7H_{16} ; [142-85-5]
Octane; C_8H_{18} ; [111-65-9]
Nonane; C_9H_{20} ; [111-84-2]
Decane; $C_{10}H_{22}$; [124-18-5]
Undecane; $C_{11}H_{24}$; [1120-21-4]
Dodecane; $C_{12}H_{26}$; [112-40-3]
Tridecane; $C_{13}H_{28}$; [629-50-5]
Tetradecane; $C_{14}H_{30}$; [629-59-4]
Pentadecane; $C_{15}H_{32}$; [629-62-9]
Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:
P. J. Hesse, R. Battino, P. Scharlin, and E. Wilhem, J. Chem. Eng. Data **41**, 195–201 (1996).

Variables:
T/K = 298.15
p_1 /MPa = 0.101325

Prepared By:
H. L. Clever

Experimental Values

Ostwald coefficient and Henry fugacity of sulfur hexafluoride at 298.15 K and a *total* pressure of 101 325 Pa. The carbon tetrafluoride mole fraction solubility at 298.15 K and a *partial* pressure of 101 325 Pa.

Alkane	Ostwald Coefficient $[L_{1,2}(T,p)]$	Henry Fugacity $10^{-6} H_{1,2}(T,p_{s,2})$/Pa	$10^4 x_1$
Hexane	0.4328	42.98	23.48
Heptane	0.3502	47.51	21.20
Octane	0.2943	51.03	19.73
Nonane	0.2578	53.04	18.98
Decane	0.2331	53.82	18.71
Undecane	0.2107	54.95	18.32
Dodecane	0.1914	56.17	17.92
Tridecane	0.1784	56.24	17.90
Tetradecane	0.1667	56.42	17.85
Pentadecane	0.1533	56.99	17.67
Hexadecane	0.1515	55.16	18.25

The refractive indices of the liquid alkanes were measured. The values were in good agreement with reliable literature values. The purities of the solvents were measured by gas chromatography and found to be greater than 99 mol % in all cases. The liquid alkanes were stored in brown glass bottles. Prior to the actual solubility measurements they were degassed by the method of Battino *et al.*[2] and transferred into the apparatus under their own vapor pressure.
Alkane properties listed and used by the authors are given below (see paper for references).

1	2	3	4	5	6	7	8	9	10
Hexane	20179	0.6549	1.387	1669	247.8	0.299	507.90	3.035	369.9
Heptane	6104	0.6795	1.252	1438	259.6	0.350	540.15	2.735	430.1
Octane	1875	0.6985	1.155	1282	268.6	0.397	568.95	2.490	492.4
Nonane	584	0.7138	1.088	1175	276.1	0.443	594.90	2.290	555.2
Decane	183	0.7264	1.042	1094	284.0	0.490	617.65	2.105	624.1
Undecane	58	0.7365	1.004	1031	290.3	0.533	638.85	1.955	688.6
Dodecane	19	0.7452	0.976	988	294.5	0.573	658.65	1.830	753.7
Tridecane	6	0.7527	0.951	988	299.1	0.618	676	1.710	823.1
Tetradecane	2	0.7592	0.929	910	304.4	0.654	693	1.610	823.1
Pentadecane	>1	0.7649	0.911	882	308.0	0.696	708	1.515	965.5
Hexadecane	>1	0.7699	0.895	857	311.4	0.737	722	1.435	1034.0

A key to the column headings is given on the following page.

Column	Property	Column	Property
1	Alkane	6	Internal pressure, $10^{-6}\Pi_2{}^{L}$/Pa
2	Vapor pressure, $p_{s,2}$ /Pa	7	Acentric factor, ω_2
3	Density, $10^{-3}\rho_2{}^{L}$/(kg m^{-3})	8	Critical temperature, $T_{c,2}$ /K
4	Isobaric expansivity, $10^{3}\alpha_{p,2}{}^{L}$/K^{-1}	9	Critical pressure, $10^{-6}p_{c,2}$ /Pa
5	Isothermal compressibility, $10^{12}\beta_{T,2}{}^{L}$/Pa^{-1}	10	Critical molar volume, $10^{6}V_{c,2}$ /(m^3 mol^{-1})

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were measured with a Ben-Naim/Baer type apparatus as modified by the author.[1] The apparatus has four equilibration cells of ~26, 65, 380, and 1650 cm^3 volume for different ranges of Ostwald coefficients. The equilibration vessels and the gas burets were calibrated with doubly distilled water, and the respective volumes are known to ±0.01 cm^3. The total pressure was determined with a pressure transducer. The entire apparatus is in a large air thermostat controlled to better than ±0.01 K. Temperatures were measured by a calibrated platinum resistance cell based on IPTS-68. Prior to measurement the solvents were degassed by the method of Battino *et al.*[2] and transferred under their own vapor pressure into the solubility apparatus.

Source and Purity of Material:

(1) Carbon tetrafluoride. Either Airco or Matheson. Minimum mole percent purity stated to be 99.7%.
(2) Alkanes.
Hexane: Fisher Scientific, >99 mol %
Heptane: Philips Petroleum, >99 mol %
Octane: General Dynamics, >99 mol %
Nonane: Philips Petroleum, >99 mol %
Decane: Philips Petroleum, >99 mol %
Undecane: Philips Petroleum, >99 mol %
Dodecane: Philips Petroleum, >99 mol %
Tridecane: Alfa Products, >99 mol %
Tetradecane: Philips Petroleum, >99 mol %
Pentadecane: Alfa Products, >99 mol %
Hexadecane: Philips Petroleum, >99 mol %

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.002 (authors).

References:
[1]T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[2]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Heptane; C_7H_{16} ; [142-82-5]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 277.95–307.08
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	10^3x_1	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
4.80	277.95	2.257	0.352	0.358
14.77	287.92	2.193	0.338	0.356
26.99	300.14	2.140	0.325	0.357
33.93	307.08	2.112	0.316	0.358

The compiler calculated the Bunsen and Ostwald coefficients values assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 277.95 K and 307.08 K: $\ln x_1 = -6.7882 + 1.9250(T/100\ \mathrm{K})$
The standard error about the regression line is 5.70×10^{-6}, calculated (smoothed) solubilities are given below.

T/K	10^2x_1
278.15	2.252
288.15	2.198
298.15	2.149
308.15	2.105

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2 , evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilibration is attained within 24 h.

Source and Purity of Material:

(1) Tetrafluoromethane. Matheson Co., Inc. Stated to be minimum purity of 95 mol %, further purified by multiple trap distilltion.
(2) Heptane. Fisher Co. Spectroanalytical grade. Dried with Drierite and distilled.

Estimated Error:
$\delta x_1/x_1$ = ±0.002 (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Tetrafluoroethane; CF_4; [75-73-0]
(2) Octane; C_8H_{18}; [111-65-9]

Original Measurements:
E. Wilhelm and R. Battino, J. Chem. Thermodyn. **3**, 379–392 (1971).

Variables:
T/K = 297.48–308.51
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
297.48	19.65	0.270	0.2941
297.56	19.68	0.271	0.2947
308.50	19.71	0.267	0.3020
308.51	19.57	0.266	0.3000

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.

Smoothed data for use between 297.48 K and 308.51 K: $\ln x_1 = -6.2673 + 0.1066(T/100\ \mathrm{K})$

The standard error about the regression line is 7.16×10^{-6}, and smoothed solubilities are:

T/K	$10^4 x_1$
298.15	19.66
303.15	19.65
313.15	19.64

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]

Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.

Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Purity better than 99 mol %.
(2) Octane. Phillips Petroleum Co. Fractionally distilled through a packed vacuum jacketed 1 m column at a reflux ratio of 20 or better.

Estimated Error:
$\delta L/L = \pm 0.01$

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) 2,2,4-Trimethylpentane (*iso*-octane); C_8H_{18}; [540-84-1]

Original Measurements:
P. J. Hesse, R. Battino, P. Scharlin, and E. Wilhelm, J. Chem. Thermodyn. **31**, 1175–1181 (1999).

Variables:
T/K = 298.15
p_1 /Pa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	Ostwald Coefficient ($L_{1,2}$ /cm^3 cm^{-1})	Henry's Constant [$10^{-6}H_{1,2}(T,p_{s,2})$/Pa]	$10^4 x_1$
298.15	0.3851	38.37	26.25

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was measured with a Ben-Naim Baer type apparatus as modified by Tominaga *et al.*[1] The apparatus had several equilibration chambers from 26 to 1650 cm^3 to cover a large range of Ostwald Coefficient values. The equilibration vessels and the gas burets were calibrated with double distilled water and the volumes are known to ± 0.01 cm^3. Gas volumes were determined using a microprocessor that counted the number of steps on a stepping motor which advanced a precision screw which moved in a close-fitting piston. The volumes were determined to a few parts per thousand. The pressure was measured with a pressure transducer and was kept nulled to within one part per thousand. A typical dissolution time to a stable equilibrium point was about 3 h. Prior to the measurement the solvent was degassed by the method of Battino *et al.*[2] and transferred under its own vapor pressure into the solubility apparatus.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson or Airco. Used as received. Stated to be of 0.9999 minimum mass fraction purity.
(2) 2,2,4-Trimethylpentane or isooctane. Philips Petroleum. R. I. (n_D) agreed well with accepted literature value. GLC found a purity of >0.99 mass fraction.

Estimated Error:
δT/K = ± 0.05
$\delta p/p = \pm 0.001$
$\delta x_1/x_1 = \pm 0.002$
Author's estimates.

References:
[1]T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Cheng. Eng. Data **31**, 175 (1986).
[2]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 2,2,4-Trimethylpentane or *iso*-octane; C_8H_{18} ; [540-84-1]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 277.80–308.83
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in 2,2,4-trimethylpentane at a partial pressure of 101.325 kPa between 277.80 K and 308.83 K

t/°C	T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP)cm^3 atm^1]	Ostwald Coefficient (L/cm^3 cm^{-3})
4.65	277.80	31.61	0.438	0.455
14.55	287.70	30.10	0.412	0.434
24.50	297.65	29.23	0.396	0.432
35.68	308.83	38.01 [*sic*]	—	—

The compiler calculated the Bunsen and Ostwald coefficient values assuming ideal gas behavior.

Smoothed data for use between 277.80 K and 308.83 K. The value at 308.83 K was used as 28.01×10^{-4}. The smoothed data treatment results in the following equation: $\ln x_1 = -6.9356 + 3.2669/(T/100\ \mathrm{K})$.

The standard error about the regression line is 3.86×10^{-6}, and the smoothed data are:

T/K	$10^4 x_1$
278.15	31.48
288.15	30.22
298.15	29.09
308.15	28.08

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C, the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid nitrogen, then evacuating and then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements in the buret before and after introduction of gas into the pipet. The stirrer is set in motion. Equilibration is attained within 24 h.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Minimum specified purity 95 mol %. Purified further by multiple trap distillations.
(2) 2,2,4-Trimethylpentane. Phillips Petroleum Co. Dried with anhydrous magnesium perchlorate and fractionally distilled.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.002$ (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Octane; C_8H_{18} ; [111-65-9]
(2) Decane; $C_{10}H_{22}$; [124-18-5]

Original Measurements:
R. J. Wilcock, R. Battino, W. F. Danforth, and E. Wilhelm, J. Chem. Thermodyn. **10**, 817–822 (1978).

Variables:
T/K = 283.21–298.21
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
		Octane	
283.21	20.47	0.2849	0.2954
298.21	20.00	0.2738	0.2989
		Decane	
298.12	18.73	0.2139	0.2335

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]

Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.

Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.7 mol %.
(2) Octane. Phillips Petroleum Co. Stated to be 90 mol %, distilled, density at 298.15 K, ρ/g cm^{-3} = 0.6988.
(2) Decane. Phillips Petroleum Co. Stated to be 90 mol %, distilled, density at 298.15 K, ρ/g cm^{-3} = 0.7264.

Estimated Error:
ρT/K = ±0.02
ρp/mmHg = ±0.5
$x_1 / x_1 = \pm 0.01$

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]

Original Measurements:
J. Dymond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130–131 (1961).

Variables:
T/K = 298.15
p_1 /kPa = 101.325

Prepared By:
A. L. Cramer and H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
298.15	10.30	0.212	0.232

The compiler calculated the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consists of an all-glass buret system and a two bulb absorption vessel.

A magnetic pump forces solvent from a lower bulb over the wall of the upper bulb which contains the gas. The solvent flows back into the lower bulb. Pumping is continued until there is no further pressure change.

The amount of gas absorbed is calculated from the initial and final gas pressure.

Source and Purity of Material:
(1) Tetrafluoromethane. Nothing specified.
(2) Cyclohexane. Nothing specified.

Estimated Error:
δT/K = ±0.05
$\delta x_1 / x_1$ = ±0.01 or less.

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 278.14–308.15
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in cyclohexane at a partial pressure of 101.325 kPa from 278.14 K to 308.15 K

t/°C	T/K	$10^4 / x_1$	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
4.99	278.14	10.22	0.216	0.220
14.83	287.98	10.24	0.214	0.226
24.69	287.98	10.32	0.213	0.232
35.00	287.96	10.32	0.213	0.240

The compiler calculated the Bunsen and Ostwald coefficient values, assuming an ideal gas.
Smoothed data for use between 278.14 K and 308.15 K, $\ln x_1 = -6.6775 - 0.5867/(T/100\ \mathrm{K})$.
The standard error about the regression line is 3.41×10^{-6}, and the smoothed solubilities are:

T/K	$10^4 x_1$
278.15	10.12
288.15	10.27
298.15	10.34
308.15	10.41

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C, the pipet at any temperature from 5 to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid nitrogen, then evacuating and then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements in the buret before and after introduction of gas into the pipet. The stirrer is set in motion. Equilibration is attained within 24 h.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Minimum specified purity 95 mol %. Purified further by multiple trap distillations.
(2) Cyclohexane. Eastman Organic Chemical Co. Analytical reagent grade. Dried with Drierite and distilled.

Estimated Error:
$\delta x_1 / x_1$ = ±0.002 (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

Original Measurements:
L. R. Field, E. Wilhelm, and R. Battino, J. Chem. Thermodyn. **6**, 237–243 (1974).

Variables:
T/K = 284.40–313.25
p/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
284.40	12.97	0.230	0.2397
298.20	13.71	0.239	0.2615
313.25	13.26	0.228	0.2613

The authors adjusted the gas solubility values to a gas partial pressure of 101.325 kPa (1 atm) by Henry's law. The compiler calculated the Bunsen coefficients.

Smoothed data for use between 284.40 K and 313.25 K: $\ln x_1 = -6.3913 - 0.6874/(T/100\ \mathrm{K})$.

The standard error about the regression line is 4.86×10^{-5}, and the smoothed solubilities are:

T/K	$10^4 x_1$
283.15	13.15
293.15	13.26
298.15	13.31
303.15	13.36
313.15	13.41

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billet[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred and the vacuum applied intermittently through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm. Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas and solvent vapor at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volume in the buret system. The solvent is collected in a tared flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Either Matheson Co. or Air Products and Chemicals Co. Purest grade available, minimum purity greater than 99 mole %.
(2) Methylcyclohexane. Phillips Petroleum. Pure grade. Distilled.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morission and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and F. D. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) *cis*-1,2-Dimethylcyclohexane; C_8H_{16}; [2207-01-4]

Original Measurements:
E. B. Geller, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **8**, 197–202 (1976).

Variables:
T/K = 297.90, 312.99
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
297.90	12.54	0.1987	0.2167
312.99	12.38	0.1931	0.2213

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.

Smoothed data for use between 297.90 K and 312.99 K: $\ln x_1 = -6.9546 + 0.8145/(T/100\ \mathrm{K})$.

T/K	$10^4 x_1$
298.15	12.57
308.15	12.43

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.7 mol %.
(2) *cis*-1,2-Dimethylcyclohexane. Chemical Samples Co. Fractionally distilled and stored in the dark. Refractive index (NaD, 298.15 K) 1.4337.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) *trans*-1,2-Dimethylcyclohexane; C_8H_{16} ; [6876-23-9]

Original Measurements:
E. B. Geller, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **8**, 197–202 (1976).

Variables:
T/K = 298.07, 313.03
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
298.07	14.92	0.2304	0.2514
313.03	14.86	0.2261	0.2591

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data—the equation is based on only two points and should be used with caution.
For use between 298.07 K and 313.03 K: $\ln x_1 = -6.6009 + 0.2794/(T/100\ \mathrm{K})$.

T/K	$10^4 x_1$
298.15	14.93
308.15	14.88

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.7 mol %.
(2) *trans*-1,2-Dimethylcyclohexane. Chemical Samples Co. Fractionally distilled and stored in the dark. Refractive index (NaD, 298.15 K) 1.4248.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) *trans*-1,3-Dimethylcyclohexane; 41 mol %; C_8H_{16} ; [2207-03-6]
(3) *cis*-1,3-Dimethylcyclohexane, 59 mol %; C_8H_{16} ; [638-04-0]

Original Measurements:
E. B. Geller, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **8**, 197–202 (1976).

Variables:
T/K = 298.11, 312.98
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
298.11	15.19	0.2338	0.2552
312.98	14.99	0.2273	0.2604

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior. The solubility values were adjusted to a tetrafluoromethane partial pressure of 101.325 kPa by Henry's law.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.7 mol %.
(2) *trans*-1,3-Dimethylcyclohexane.
(3) *cis*-1,3-Dimethylcyclohexane. Chemical Samples Co. Purchased as binary mixture, used as received. Authors analyzed mixture by refractive index.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) *trans*-1,4-Dimethylcyclohexane; 30 mol %; C_8H_{16}; [2207-04-7]
(3) *cis*-1,4-Dimethylcyclohexane, 70 mol %; C_8H_{16}; [624-29-3]

Original Measurements:
E. B. Geller, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **8**, 197–202 (1976).

Variables:
T/K = 298.07,313.12
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
298.07	15.11	0.2334	0.2547
313.12	14.86	0.2256	0.2586

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior. The solubility values were adjusted to a tetrafluoromethane partial pressure of 101.325 kPa by Henry's law.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.7 mol %.
(2) *trans*-1,4-Dimethylcyclohexane.
(3) *cis*-1,4-Dimethylcyclohexane. Chemical Samples Co. Purchased as binary mixture, used as received. Authors analyzed mixture by refractive index.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetraffuoromethane; CF_4; [75-73-0]
(2) Cyclooctane; C_8H_{16}; [292-64-8]

Original Measurements:
R. J. Wilcock, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **9**, 111–115 (1977).

Variables:
T/K = 289.11–313.43
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
289.11	6.43	0.1074	0.1272
298.23	6.74	0.1116	0.1219
313.43	7.79	0.1272	0.1219

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 288.15 K and 313.15 K: $\ln x_1 = -4.8370 - 7.2965/(T/100\ \mathrm{K})$
The standard error about the regression line is 1.58×10^{-5}, and smoothed solubilities follow.

T/K	$10^4 x_1$
288.15	6.30
298.15	6.86
308.15	7.43

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Products and Chemicals, Inc. Minimum mole % purity is 99.7.
(2) Cyclooctane. Chemical Samples Co. 99 mole %, distilled, refractive index (NaD, 298.15 K) 1.4562.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:
D. F. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753–760 (1971).

Variables:
T/K = 287.88–297.24
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
14.73	287.88	5.00	0.127	0.1339
14.80	287.95	4.93	0.125	0.1319
23.28	296.43	5.26	0.132	0.1435
23.28	296.74	5.32	0.134	0.1452
24.09	296.74	5.31	0.133	0.1450

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 287.88 K and 298.15 K: $\ln x_1 = -5.4564 - 6.1937/(T/100\ \text{K})$.
The standard error about the regression line is 3.44×10^{-6}, and smoothed solubilities follow.

T/K	$10^4 x_1$
283.15	4.79
288.15	4.97_5
293.15	5.16
298.15	5.35

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Either Air Products and Chemicals Inc. or the Matheson Co., Inc. Purest grade available. Minimum purity 99.0 mole % (usually >99.9 mol %).
(2) Benzene. Mallinkrodt Co. Thiophene free, analytical reagent grade. Used as received.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-2]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K = 280.82–305.66
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
5.96	279.11	5.41	0.139	0.142
14.76	287.91	5.57	0.141	0.149
24.78	297.93	5.71	0.143	0.156
36.20	309.35	5.96	0.147	0.166

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 279.11 K and 309.35 K: $\ln x_1 = -6.5541 + 2.7057/(T/100\ \text{K})$.
The standard error about the regression line is 2.86×10^{-6} and the smoothed solubilities are:

T/K	$10^4 x_1$
278.15	5.39
288.15	5.57
298.15	5.75
298.15	5.92

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C; the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid N_2, evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet, and boiled again for final degassing. The solvent never comes into contact with stopcock grease. It is sealed off by mercury. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements. The mixture is stirred, equilbration is attained within 24 h.

Source and Purity of Materials:
(1) Tetrafluoromethane. Matheson Co., Inc. Stated to be minimum purity of 95 mol %, further purified by by multiple trap distillation.
(2) Benzene. Brothers Chemical Co. Analytical reagent grade. Shaken successively with concertration H_2SO_4, 5% NaOH solution and water (twice). Dried over Oronite and distilled.

Estimated Error:
$\delta x_1 / x_1$ = ±0.002 (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Methylbenzene or toluene; C_7H_8 ; [108-88-3]

Original Measurements:
L. R. Field, E. Wilhelm, and R. Battino, J. Chem. Thermodyn. **6**, 237–243 (1974).

Variables:
T/K = 283.46–313.40
p/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
283.46	6.16	0.131	0.1363
297.58	6.93	0.145	0.1585
313.40	6.82	0.145	0.1615

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed Data for use between 283.46 K and 313.40 K: $\ln x_1 = -6.3074 - 3.0112/(T/100\ \mathrm{K})$.
The standard error about the regression line is 3.68×10^{-5}, and smoothed solubilities are:

T/K	$10^4 x_1$
283.15	6.29
293.15	6.53
298.15	6.64
303.15	6.75
313.15	6.97

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred and the vacuum applied intermittently through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas and solvent vapor at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volume in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Either Matheson Co. or Air Products and Chemicals Co. Purest grade available, minimum purity greater than 99 mole %.
(2) Methylbenzene. Phillips Petroleum. Pure grade. Distilled.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morission and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and F. D. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1,2-Dimethylbenzene or *o*-xylene; C_8H_{10} ; [95-47-6]

Original Measurements:
J. E. Byrne, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **7**, 515–522 (1975).

Variables:
T/K = 283.22–313.17
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
283.22	6.34	0.1159	0.1234
283.37	6.37	0.1194	0.1239
298.17	6.43	0.1190	0.1299
313.11	6.61	0.1207	0.1383
313.17	6.59	0.1207	0.1379

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 283.15 K and 313.15 K: $\ln x_1 = -6.9672 - 1.1202/(T/100\ \mathrm{K})$.
The standard error about the regression line is 1.25×10^{-5}, and the smoothed solubilities are:

T/K	$10^4 x_1$
283.15	6.34
293.15	6.43
298.15	6.47
303.15	6.52
313.15	6.59

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Either Air Products and Chemicals, Inc. or Matheson Co. Inc. 99 mole % or better.
(2) 1,2-Dimethylbenzene. Phillips Petroleum Co. Pure grade.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1,3-Dimethylbenzene or *m*-xylene; C_8H_{10} ; [108-38-3]

Original Measurements:
J. E. Byrne, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **7**, 515–522 (1975).

Variables:
T/K = 283.11–313.75
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
283.11	7.35	0.1355	0.1404
283.22	7.32	0.1349	0.1399
298.16	7.52	0.1273	0.1490
313.75	7.57	0.1352	0.1553

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 283.11 K and 313.75 K: $\ln x_1 = -6.8752 - 0.9654/(T/100\ \mathrm{K})$.
The standard error about the regression line is 4.19×10^{-6}, and the smoothed solubilities are:

T/K	$10^4 x_1$
283.15	7.35
293.15	7.43
298.15	7.47
293.15	7.51
313.15	7.59

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Either Air Products and Chemicals, Inc. or Matheson Co. Inc. 99 mole % or better.
(2) 1,3-Dimethylbenzene. Phillips Petroleum Co. Pure grade.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.005

References:
[1]J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968)
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1,4-Dimethylbenzene or *p*-xylene; C_8H_{10} ; [106-42-3]

Original Measurements:
J. E. Byrne, R. Battino, and E. Wilhelm, J. Chem. Thermodyn. **7**, 515–522 (1975).

Variables:
T/K = 287.95–313.18
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
287.95	7.67	0.1403	0.1479
288.16	7.62	0.1392	0.1469
298.16	7.78	0.1407	0.1536
313.13	7.90	0.1409	0.1615
313.18	7.93	0.1414	0.1621

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 287.95 K and 313.18 K: $\ln x_1 = -6.7451 + 1.2402/(T/100\ \mathrm{K})$.
The standard error about the regression line is 2.70×10^{-6}, and the smoothed solubilities are:

T/K	$10^4 x_1$
293.15	7.71
298.15	7.76
303.15	7.82
313.15	7.92

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Either Air Products and Chemicals, Inc. or Matheson Co., Inc. 99 mole % or better.
(2) 1,4-Dimethylbenzene. Phillips Petroleum Co. Pure grade. Used as received.

Estimated Error:
δT/K = ±0.01
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc.2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:

(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1-Alkanoles (C_1 to C_{11})
Methanol; CH_3OH; [67-56-1]
Ethanol; C_2H_5OH; [64-17-5]
1-Propanol; C_3H_7OH; [71-23-8]
1-Butanol; C_4H_9OH; [71-36-3]
1-Pentanol; $C_5H_{11}OH$; [71-41-0]
1-Hexanol; $C_6H_{13}OH$; [111-27-3]
1-Heptanol; $C_7H_{15}OH$; [111-70-6]
1-Octanol; $C_8H_{17}OH$; [111-87-5]
1-Nonanol; $C_9H_{19}OH$; [143-08-8]
1-Decanol; $C_{10}H_{21}OH$; [112-30-1]
1-Undecanol; $C_{11}H_{23}OH$; [112-42-5]

Original Measurements:

S. Bo, R. Battino, and E. Wilhelm, J. Chem. Eng. Data **38**, 611–616 (1993).

Variables:

T/K=298.15
p_1 /MPa=0.101325

Prepared By:

H. L. Clever

Experimental Values

Ostwald coefficient and Henry fugacity of tetrafluoromethane at 298.15 K and a *total* pressure of 101 325 Pa. The sulfur hexafluoride mole fraction solubility at 298.15 K and a *partial* pressure of 101 325 Pa

Alkanol	Ostwald Coefficient $L_{1,2}(T,p)$	Henry Fugacity $[10^{-6}H_{1,2}(T,p_{s,2})/\mathrm{Pa}]$	10^4x_1
Methanol	0.1855	324.5	3.110
Ethanol	0.1917	218.1	4.620
1-Propanol	0.1731	188.6	5.338
1-Butanol	0.1580	168.9	5.962
1-Pentanol	0.1401	161.2	6.245
1-Hexanol	0.1303	150.4	6.696
1-Heptanol	0.1218	142.2	7.083
1-Octanol	0.1135	136.5	7.375
1-Nonanol	0.1079	130.1	7.741
1-Decanol	0.1014	126.5	7.961
1-Undecanol	0.09624	122.8	8.199

Alkanol properties listed and used by the authors. See paper for references.

1	2	3	4	5	6	7	8	9	10
Methanol	16941	0.7866	1.195	1348	285	0.564	512.3	8.092	117.8
Ethanol	7876	0.7851	1.093	1153	281	0.643	514.1	6.140	166.9
1-Propanol	2786	0.7996	0.995	1006	295	0.620	536.7	5.168	218.5
1-Butanol	858	0.8058	0.932	942	295	0.591	562.4	4.418	218.5
1-Pentanol	259	0.8111	0.893	884	301	0.579	588.0	3.868	326.5
1-Hexanol	77	0.8154	0.870	836	310	0.575	611.0	3.413	393.0
1-Heptanol	22	0.8194	0.861	800	321	0.580	632.5	3.058	393.0
1-Octanol	6	0.8218	0.854	777	328	0.594	652.6	2.777	506.7
1-Nonanol	2	0.8245	0.826	752	327	0.610	670.5	2.546	572.4
1-Decanol	>1	0.8266	0.812	733	330	0.629	687.1	2.330	648.7
1-Undecanol	>1	0.8292	0.813	723	335	0.656	703.3	2.147	718.0

The definitions of each column heading follows:
1. Alkane
2. Vapor pressure, $p_{s,2}$ /Pa
3. Density, $10^{-3}\rho_2{}^{L}$/(kg m^{-3})
4. Isobaric expansivity, $10^3\alpha_{p,2}{}^{L}$/K^{-1}
5. Isothermal compressibility, $10^{12}\beta_{T,2}{}^{L}$/Pa^{-1}
6. Internal pressure, $10^{-6}\Pi_2{}^{L}$/Pa
7. Acentric factor, ω_2
8. Critical temperature, $T_{c,2}$/K
9. Critical pressure, $10^{-6}p_{c,2}$ /Pa
10. Critical molar volume, $10^6V_{c,2}$ /(m^3 mol^{-1})

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were measured with a Ben-Naim/Baer type apparatus as modified by the authors.[1] The apparatus has four equilibration cells of ~26, 65, 380, and 1650 cm^3 volume for different ranges of Ostwald coefficients. The equilibration vessels and the gas burettes were calibrated with doubly distilled water, and the respective volumes are known to ±0.01 cm^3. The total pressure was determined with a pressure transducer. The entire apparatus is in a large air thermostat controlled to better than ±0.01 K. Temperatures were measured by a calibrated platinum resistance cell based on IPTS-68. Prior to measurement the solvents were degassed by the method of Battino *et al.*[2] and transferred under their own vapor pressure into the solubility apparatus.

Source and Purity of Materials:

(1) Tetrafluoromethane. Either Matheson or Airco. Minimum mole % purity stated to be 99.7.
(2) 1-Alkanols.
Methanol; Fisher Certified grade.
Ethanol; Pharmco (USP 200 Proof)
1-Propanol; Fisher Certified grade. (99.8%)
1-Butanol; Fisher Certified grade.
1-Pentanol; Fisher Certified grade. (99.3%)
1-Hexanol; Fisher Certified grade. (99.6%)
1-Heptanol; Fisher Certified grade. (99.6%)
1-Octanol; Fisher Certified grade. (99.3%)
1-Nonanol; Fluka.
1-Decanol; Fluka.
1-Undecanol; Fluka.
All alkanols were distilled at least once through a 1.2 m vacuum jacketed packed column at a reflux ratio of 15 or better. The middle 80% of the distillate was used for the solubility measurements. The refractive index of each purified alkanol agreed well with reliable literature values. The purities were determined by gas chromatography.

Estimated Error:

δT/K=±0.1
$\delta x_1/x_1$=±0.002 (authors).

References:

[1]T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[2]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1-Propanol; C_3H_8O; [71-23-8]

Original Measurements:
V. G. Komarenko and V. G. Manzhelii, Ukr. Fiz. Zh. (Ukr. Ed.) **13**, 387–391 (1968); *Ukr. Phys. J. (Engl. Transl.) **13**, 273–276 (1968).

Variables:
T/K = 173.15–243.15
p_1 /kPa = 26.664 (200 mmHg)

Prepared By:
H. L. Clever

Experimental Values

Solubility of CF_4 in 1-propanol between 173.15 K and 243.15 K at partial pressures of 26.664 and 101.325 kPa

t/°C	T/K	10^3x_1 (p_1 /mmHg = 200)	10^3x_1 (p_1 /mmHg = 760)
−100	173.15	0.569	2.16
−90	183.15	0.452	1.72
−80	193.15	0.396	1.50
−70	202.15	0.335	1.273
−60	213.15	0.281	1.068
−50	223.15	0.225	0.855
−40	233.15	0.1955	0.743
−30	243.15	0.1698	0.645

The compiler added the Kelvin temperatures and calculated the mole fraction solubility values at 101.325 kPa (760 mmHg) assuming that Henry's law is obeyed.

Auxiliary Information

Method/Apparatus/Procedure:
The solvent was degassed by vacuum. A thin layer of alcohol, cooled to 125–175 K, was kept for 20 h in a vacuum maintained at 10^{-3} mmHg.
The degassed liquid was sealed under vacuum in an ampoule which was placed in the apparatus. The apparatus consisted of a manometer, a mercury compesator, and a solubility cell divided by a mercury seal. A gas pressure of 200 mmHg and the temperature were established. The foil ends of the ampoule were pierced. The gas dissolved as the liquid flowed through a series of small cups. The amount of gas dissolved was measured by the rise in mercury level in the compensator. Some measurements were made at 400 mm Hg gas pressure. The results confirmed that Henry's law is obeyed.

Source and Purity of Material:
(1) Tetrafluoromethane. Source not specified. Purity by chromatographic method was 99.93%.
(2) 1-Propanol. Purified and analyzed in the All Union Sci. Res. Inst. For Single Crystals and High Purity Substances. Purity stated to be 99.97 mass %.

Estimated Error:
δT/K = ±0.05
δp_1 /mmHg = ±0.01
$\delta x_1 / x_1$ = ±0.005

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

Original Measurements:
J. Pardo, M. C. Lopez, J. Santafe, F. M. Royo, and J. S. Urieta, Fluid Phase Eq. **109**, 29–37 (1995).

Variables:
T/K = 263.15–303.15
p_1 /kPa = 101.33

Prepared By:
H. L. Clever

Experimental Values

T/K	10^4x_1	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
263.15	6.318	0.1591	0.1533
273.15	6.190	0.1545	0.1545
283.15	6.055	0.1497	0.1552
293.15	5.857	0.1435	0.1540
298.15	5.797	0.1414	0.1543
303.15	5.711	0.1386	0.1538

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -8.1409 + 205.091/(T/\mathrm{K})$ ($\sigma = 0.0061$).
From the equation they obtained ΔH°_1 /kJ mol^{-1} = −1.71 and ΔS°_1 /J K^{-1} mol^{-1} = −68 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) 1-Butanol. Aldrich Chemical Co. Purity checked by GLC to be 99.8%.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 2-Butanol; $C_4H_{10}O$; [78-92-2]

Original Measurements:
J. Pardo, M. C. Lopez, J. A. Mayoral, F. M. Royo, and J. S. Urieta, Fluid Phase Eq. **134**, 133–140 (1997).

Variables:
T/K = 263.15–303.15
p_1 /kPa = 101.33

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
263.15	7.693	0.1939	0.1868
273.15	7.357	0.1835	0.1835
283.15	7.105	0.1753	0.1817
293.15	6.939	0.1694	0.1818
298.15	6.799	0.1651	0.1802
303.15	6.693	0.1617	0.1794

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -8.1950 + 268.754/(T/\mathrm{K})$ ($\sigma = 0.0050$).
From the equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −2.23 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −68 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction value is calculated from the author's smoothing equation. The other values are from the Table in the paper.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) 2-Butanol. Aldrich Chemical Co. Purity checked by GLC to be 99%.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-2]

Original Measurements:
J. Pardo, M. C. Lopez, J. Santafe, F. M. Royo, and J. S. Urieta, Fluid Phase Eq. **119**, 165–173 (1997).

Variables:
T/K = 263.15–303.15
p_1 /kPa = 101.33

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
263.15	8.173	0.2040	0.1965
273.15	7.786	0.1925	0.1925
283.15	7.446	0.1823	0.1890
293.15	7.189	0.1744	0.1872
298.15	7.058	0.1704	0.1860
303.15	6.652	0.1670	0.1860

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -8.3405 + 323.301/(T/\mathrm{K})$ ($\sigma = 0.0036$).
From the equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −2.69 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −69 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction value is calculated from the author's smoothing equation. The other values are from the Table in the paper.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) 2-Methyl-1-propanol. Aldrich Chemical Co. Purity checked by GLC to be 99.5%.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) 1-Octanol; $C_8H_{17}O$; [111-87-5]

Original Measurements:
R. J. Wilcock, R. Battino, W. F. Danforth, and E. Wilhelm, J. Chem. Thermodyn. **10**, 817–822 (1978).

Variables:
T/K = 282.66–313.48
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
282.66	7.022	0.1003	0.1038
298.15	7.121	0.1005	0.1097
313.48	7.298	0.1017	0.1167

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 283.15 K and 313.15 K: $\ln x_1 = -6.8736 - 1.1014/(T/100\ \mathrm{K})$.
The standard error about the regression line is 3.72×10^{-6}, and smoothed data follow.

T/K	$10^4 x_1$
283.15	7.013
293.15	7.107
298.15	7.152
303.15	7.195
313.15	7.279

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]

Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.

Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.7 mol %.
(2) 1-Octanol. Eastman Organic Chemicals. Distilled, density at 298.15 K, ρ/g cm^{-3} = 0.8247.

Estimated Error:
δT/K = ±0.02
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) 1-Decanol; $C_{10}H_{21}O$; [112-30-1]

Original Measurements:
R. J. Wilcock, R. Battino, W. F. Danforth, and E. Wilhelm, J. Chem. Thermodyn. **10**, 817–822 (1978).

Variables:
T/K = 282.61–313.37
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
282.61	7.747	0.0915	0.09463
298.31	7.845	0.0915	0.09996
313.37	7.948	0.0916	0.1051

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 283.15 K and 313.15 K: $\ln x_1 = -6.8736 - 1.1014/(T/100\ \mathrm{K})$.
The standard error about the regression line is 7.45×10^{-7}.

T/K	$10^4 x_1$
283.15	7.748
293.15	7.817
298.15	7.850
303.15	7.882
313.15	7.943

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]

Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.

Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Products and Chemicals Inc. Minimum mole fraction purity stated to be 99.7 mol %.
(2) 1-Decanol. Eastman Organic Chemicals. Distilled, density at 298.15 K, ρ/g cm^{-3} = 0.8206.

Estimated Error:
δT/K = ±0.02
δp/mmHg = ±0.5
$\delta x_1 / x_1$ = ±0.01

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

Original Measurements:
M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. Phys. Biol. **80**, 621–625 (1983).

Variables:
T/K = 285.15–303.15
p_1 /kPa = 101

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in 1,4-dioxane at a partial pressure of 101 kPa between 285.15 K and 303.15 K

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
285.15	3.22_6	0.08560	0.08935
289.15	3.30_2	0.08725	0.08935
293.15	3.36_0	0.08840	0.09485
298.15	3.41_7	0.08940	0.09755
303.15	3.46_8	0.08930	0.10015

The compiler calculated the Bunsen and the Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior. The values were rounded to the nearest 0.00005.

The authors fitted their data to the equation: $-\ln x_1 = -1.162 \ln(T/\mathrm{K}) + 14.605$

from which they obtained $\Delta H°_1$ /kJ mol^{-1} = 2.88 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −57 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer.[1] It was described in detail in an earlier paper of the authors.[2]

The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent saturated gas.

Literature 1,4-dioxane vapor pressures were fitted to the equation: $\ln(p_2/\mathrm{kPa}) = -4591.3/(T/\mathrm{K}) + 16.98$.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) 1,4-Dioxane. Merck and Co. Purity checked by GLC to be >99%.

Estimated Error:
δT/K = ±0.1
δp/kPa = ±1
$\delta x_1/x_1$ = ±0.01

References:
[1]A. Ben Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencieas Zaragoza **34**, 115–122 (1973).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Methoxybenzene (or anisole); C_7H_8; [100-66-3]

Original Measurements:
F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **78**, 171–174 (1981).

Variables:
T/K = 283.15–303.15
p_1 /kPa = 101.3

Prepared By:
C. L. Young

Experimental Values

T/K	$10^4 x_1$
283.15	3.26_1
288.15	3.31_2
293.15	3.40_8
298.15	3.45_7
303.15	3.54_1

The smoothing equation of the author is: $\ln x_1 = -1.214 \ln(T/\mathrm{K}) + 14.883$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus was similar to that used by Ben-Naim and Baer,[1] consisting essentially of a gas buret, mercury manometer, and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It appears that the mole fraction at a partial pressure of 1 atm was estimated from the raw experimental data by assuming that Henry's law is obeyed and that the partial pressure of the solvent in the gas phase is given by Raoult's law.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Purity stated to be 99 mole %.
(2) Methoxybenzene. Fluka. Purity equal to or better than 99 mole %. Checked by GC.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.04 (estimated by compiler).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Cyclopentanone; C_5H_8O; [120-92-3]

Original Measurements:
M. A. Gallardo, M. C. Lopez, J. S. Urieta, and C. Gutierrez Losa, Fluid Phase Equilib. **50**, 223–233 (1989).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
C. L. Young

Experimental Values

T/K	Henry's Coeff. 10^4 atm/$H_{2,1}$ (corrected)	Henry's Coeff. 10^4 atm/$h_{2,1}$ (uncorrected)	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	3.445	3.421	0.08838	0.08838
283.15	3.536	3.512	0.08983	0.09312
293.15	3.616	3.590	0.09090	0.09756
298.15	3.664	3.637	0.09162	0.1000
303.15	3.707	3.680	0.09223	0.1024

The compiler calculated the Bunsen and Ostwald coefficients from the author's uncorrected Henry's coefficients. See source for definition of corrected Henry's coefficient. Density data were taken from the literature.[2] Ideal gas behavior was assumed. The uncorrected column above is equal to the mole fraction solubility at 101.325 kPa. The authors fitted their data to the equation:

$$\ln(H_{2,1}/101.32\ \text{kPa}) = -7.2372 + 201.18/(T/\text{K}).$$

From the equation they obtained $\Delta H°_1$ /J mol^{-1} = 1.67 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −60 at 298.15 K and a partial pressure of 101.32 kPa.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors[1] have described their apparatus in an earlier paper. The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent saturated gas. It appears that the mole fraction solubility at 1 atm was estimated from the raw data by assuming Henry's law is obeyed and that the partial pressure of the solvent is given by Raoult's law.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) Cyclopentanone. Fluka. Purity stated to be 98.5 mole %.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.02 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]J. Timmermans, *Physico-Chemical Constants of Organic Compounds* (Elsevier, Amsterdam).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]

Original Measurements:
M. A. Gallardo, J. M. Melendo, J. S. Urieta, and C. Gutierrez Losa, Can. J. Chem. **65**, 2198–2202 (1987).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	3.77	0.0832	0.0832
283.15	3.83	0.0837	0.0868
293.15	3.90	0.0844	0.0906
298.15	3.96	0.0853	0.0931
303.15	3.97	0.0851	0.0945

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = 10.845 - 0.5278 \ln(T/\text{K})$ ($10^4\sigma = 0.013$).
From the equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −1.31 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −61 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the Table in the paper.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) Cyclohexanone. Carlo Erba. Refractive index n_D (293.15 K) = 1.45071. Purity checked by GLC to be at least 99%.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.02 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 2-Methylcyclohexanone; $C_7H_{12}O$; [583-60-8]

Original Measurements:
M. A. Gallardo, M. C. Lopez, J. S. Urieta, and C. Gutierrez Losa, Can. J. Chem. 67, 809–811 (1989).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	5.60	0.106	0.106
283.15	5.61	0.105	0.109
293.15	5.63	0.104	0.112
298.15	5.67	0.104	0.114
303.15	5.69	0.104	0.114

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -7.3332 - 42.72/(T/\mathrm{K})$ ($\sigma = 0.0021$).
From the equation, they obtained ΔH°_1 /kJ mol^{-1} = 0.36 and ΔS°_1 /J K^{-1} mol^{-1} = −61, for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer.[1] The authors have described their apparatus in an earlier paper.[2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the Table in the paper. The vapor pressure of 2-methylcyclohexanone was determined and fitted to the equation: $\ln(p_2/\mathrm{kPa}) = -5552.37/(T/\mathrm{K}) + 18.046$.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) 2-Methylcyclohexanone. Merck and Co. Refractive index n_D (293.15 K) = 1.44766. Purity checked by GLC to be at least 98.1%. Cyclo-hexanone 0.6% as impurity.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1/x_1$ = ±0.02 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735–2738 (1963).
[2]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Cycloheptanone; $C_7H_{12}O$; [502-42-1]

Original Measurements:
M. A. Gallardo, M. C. Lopez, J. S. Urieta, and C. Gutierrez-Losa, Fluid Phase Equilib. **58**, 159–172 (1990).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	3.527	0.6840	0.6840
283.15	3.645	0.7007	0.7263
293.15	3.734	0.7114	0.7635
298.15*	3.787	0.7183	0.7840
303.15	3.847	0.7264	0.8062

*Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation (see below). The other values were from the experimental data table in the paper.

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -7.0896 - 234.98/(T/\mathrm{K})$.
From the equation they obtained ΔH°_1 /kJ mol^{-1} = 1.95 and ΔS°_1 /J K^{-1} mol^{-1} = −59 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier paper.[1] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent saturated gas. It appears that the mole fraction solubility at 1 atm was estimated from the raw data by assuming Henry's law is obeyed and that the partial pressure of the solvent is given by Raoult's law.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker and Co. sample. Stated to be 99 mole %
(2) Cycloheptanone. Merck and Co. sample. Purity stated to be 99.2 mole %.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1/x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 2,6-Dimethylcyclohexanone; $C_8H_{14}O$; [2816-57-1]

Original Measurements:
M. A. Gallardo, M. C. Lopez, J. S. Urieta, and C. Gutierrez Losa, Can. J. Chem. **68**, 435–439 (1990).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	7.50	0.1239	0.1239
283.15	7.47	0.1222	0.1267
293.15	7.44	0.1207	0.1295
298.15*	7.44	0.1201	0.1311
303.15	7.43	0.1194	0.1325

*Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values are from the Table in the paper.

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -7.2901 - 25.74/(T/\mathrm{K})$ ($\sigma = 0.0006$).
From the equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −0.21 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −61 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer.[1]
The authors have described their apparatus in Carniecer *et al.*[2]
The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel.
Measurements were carried out on solvent vapor saturated gas.
Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values are from the Table in the paper.
The vapor pressure and density of 2,6-dimethyl-cyclohexanone were determined and fitted to the equations:
$\ln(p_2/\mathrm{kPa}) = -3870.53/(T/\mathrm{K}) + 12.861$ and $\rho/\mathrm{g\ cm^{-3}} = 0.9290 - 0.0008313(t/°\mathrm{C})$.

Source and Purity of Materials:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) 2,6-Dimethylcyclohexanone. Fluka. Refractive index n_D (293.15 K) = 1.44686. Purity checked by GLC to be at least 98.2%. A mixture of *E* and Z (*cis and trans*) isomers.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1/x_1$ = ±0.02 (authors).

References:
[1] A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735–38 (1963).
[2] J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1,1′-[Methylene*bis*(oxy)]*bis*ethane or formaldehyde diethyl acetal; $C_5H_{12}O_2$; [462-95-3]

Original Measurements:
L. P. Lizano, M. C. Lopez, F. M. Royo, and J. S. Urieta, J. Solution Chem. **19**, 721–728 (1990).

Variables:
T/K = 263.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever and C. L. Young

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
263.15	20.1	0.374	0.360
273.15	18.7	0.344	0.344
283.15	17.5	0.318	0.329
293.15	16.4	0.294	0.316
298.15*	16.0	0.285	0.311
303.15	15.6	0.276	0.307

*Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values are from the Table in the paper.

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior. The authors fitted their data to the equation:

$$\ln x_1 = -8.1459 + 511.78/(T/\mathrm{K}).$$

From the equation they obtained $\Delta H°_1$ /kJ mol^{-1} = −4.26 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −68 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the hypothetical unit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer.[1]
The authors have described their apparatus in Carniecer *et al.*[2]
The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel.
Measurements were carried out on solvent vapor saturated gas.
Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values are from the Table in the paper.
The vapor pressure and density of 2,6-dimethyl-cyclohexanone were determined by the authors and fitted to the equations:
$\ln(p_2/\mathrm{kPa}) = -4280.53/(T/\mathrm{K}) + 166.03$ and $\rho/\mathrm{g\ cm^{-3}} = 1134.0 - 1.0350(T/\mathrm{K})$.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99 mole %.
(2) Formaldehyde diethyl acetal. Aldrich Chem. Co. Purity checked by GLC to be at least 99%. Density and vapor pressure determined.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1/x_1$ = ±0.02 (authors).

References:
[1] A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735–38 (1963).
[2] J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).

Components:
(1)Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Tetrahydro-2-methyl-furan; $C_5H_{10}O$; [96-47-9]

Original Measurements:
F. Gibnal, M. C. Lopez, F. M. Royo. J. Pardo, and J. S. Urieta, Fluid Phase Eq. **87**, 285–294 (1993).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	9.76	0.2220	0.2220
283.15	9.75	0.2195	0.2275
293.15	9.75	0.2172	0.2331
298.15*	9.69	0.2147	0.2344
303.15	9.78	0.2147	0.2393

*Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values are from the Table in the paper.

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.
The authors fitted their data to the equation: $\ln x_1 = -6.9430 - 2.840/(T/\mathrm{K})$ $(\sigma^2 = 0.0039)$
from which they obtained $\Delta H°_1$ /kJ mol^{-1} = −0.02 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −58 for the transfer of one mole of CF_4 from the gas phase at 101 kPa to the hypotheticalunit mole fraction solution (infinitely dilute solution).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. Note that the 298.15 K mole fraction solubility value above is calculated from the authors smoothing equation. The other values were from the Table in the paper.
Vapor pressure:
$\ln(p_2/\mathrm{kPa}) = -4103.4/(T/\mathrm{K}) + 23.251$.
Density:
ρ/kg m^{-3} = 1118.3 − 0.89765(T/K).

Source and Purity of Material:
(1) Tetrafluoromethane. J. T. Baker Chemical Co. Stated to be 99%.
(2) Tetrahydro-2-methyl-furan. Fluka. R. I. n_D (293.15 K) = 1.40595. Purity checked by GLC to be > 97%. Vapor pressure and density determined and fitted to equations.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2] M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Tetrahydrofuran; C_4H_8O; [109-99-9]

Original Measurements:
F. Gibanel, M. C. Lopez, F. M. Royo, J. Santafe, and J. S. Urieta, J. Solution Chem. **22**, 211–217 (1993).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	6.19	0.1749	0.1749
283.15	6.19	0.1728	0.1791
293.15	6.20	0.1711	0.1836
298.15	6.16	0.1689	0.1844
303.15	6.21	0.1693	0.1879

The compiler calculated the Bunsen and the Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation: $\ln x_1 = -7.3962 + 2.454/(T/\mathrm{K})$ $(\sigma = 0.0000022)$
from which they obtained $\Delta H°_1$ /kJ mol^{-1} = −0.02 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −61 for the transfer of 1 mole of CF_4 from the gas phase at 101 kPa to the infinitely dilute solution.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in an earlier paper of the authors.[1,2]
The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent saturated gas.
The vapor pressure of tetrahydrofuran was determined and fitted to the equation:
$\ln(p_2/\mathrm{kPa}) = -3914.6/(T/\mathrm{K}) + 23.120$.
The density: ρ/kg m^{-3} = 1199.1 − 1.0640(T/K).

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) Tetrahydrofuran. Fluka. Purity checked by GLC to be 99.5%. R. I. n_D (293.15 K) = 1.40737.

Estimated Error:
δT/K = ±0.05 cell; ±0.2 burets.
δp/kPa = ±1
$\delta x_1 / x_1$ = ±0.01

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencieas Zaragoza **34**, 115–122 (1973).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Oxepane or hexamethylene oxide; $C_6H_{12}O$; [592-90-5]

Original Measurements:
F. Gibanel, M. C. Lopez, M. H. Gallarado, J. S. Urieta, and C. Gutierrez Losa, Fluid Phase Equilibria **42**, 261–268 (1988).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.3

Prepared By:
C. L. Young

Experimental Values

T/K	$10^4 x_1$
273.15	6.14
283.15	6.23
293.15	6.31
298.15	6.33
303.15	6.37

The smoothing equation of the author is: $\ln x_1 = 99.814 \ln(T/\mathrm{K}) - 7.0292$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus was similar to that used by Ben-Naim and Baer,[1] consisting essentially of a gas buret, mercury manometer and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It was assumed the mole fraction of solvent in the gas phase was that corresponding to the vapor pressure of the pure solvent. It appears that the mole fraction at a partial pressure of 1 atm was estimated from the raw experimental data by assuming that Henry's law is obeyed.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Purity stated to be 99 mole %.
(2) Oxepane. Merck Co. Purity stated to be 99 mole %.

Estimated Error:
δT/K = ±0.02
$\delta x_1 / x_1$ = ±0.02 (estimates by compiler).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Tetrahydro-2H-pyran; $C_5H_{10}O$; [142-68-7]

Original Measurements:
F. Gibanel, M. C. Lopez, F. M. Royo, V. Rodriguez, and J. S. Urieta, J. Solution Chem. **23**, 1247–1255 (1994).

Variables:
T/K = 273.15–303.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
273.15	7.24	0.1702	0.1702
283.15	7.31	0.1700	0.1762
293.15	7.33	0.1686	0.1809
298.15	7.37	0.1685	0.1839
303.15	7.40	0.1682	0.1867

The compiler calculated the Bunsen and the Ostwald coefficients from the authors' mole fraction values assuming ideal gas behavior.

The authors fit the data to the equation: $\ln x_1 = -7.0234 + 56.492/(T/\mathrm{K})$ $10^4\sigma^2 = 0.1$
from which they obtained: $\Delta H°_1$ /kJ mol^{-1} = −0.47 and $\Delta S°_1$ /J K^{-1} mol^{-1} = −58 for the transfer of 1 mole of CF_4 from the gas phase at 101.3 kPa to the infinitely dilute solution.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in an earlier paper of the authors.[1,2]
The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent saturated gas.
The vapor pressure of tetrahydrofuran was determined and fitted to the equation:
$\ln(p_2/\mathrm{kPa}) = -4245.4/(T/\mathrm{K}) + 23.396$.
The density: ρ/kg m^{-3} = 1173.6 − 0.9916(T/K).
Note error in density equation in the paper.

Source and Purity of Material:
(1) Tetrafluoromethane. Baker Chemical Co. Stated to be 99%.
(2) Tetrahydro-2H-pyran. Fluka. Purity checked by GLC to be 99%. R. I. n_D (293.15 K) = 1.42086.

Estimated Error:
δT/K = ±0.05 cell; ±0.2 burets.
δp/kPa = ±1
$\delta x_1 / x_1$ = ±0.007 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencieas Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Various organic solvents:
- Tri(ethylene glycol) dimethyl ether; $C_8H_{18}O_4$; [112-49-2]
- Tetra(ethylene glycol) dimethyl ether; $C_{10}H_{22}O_5$; [143-34-8]
- Dimethyl carbonate; $C_3H_6O_3$; [616-38-6]
- Diethyl carbonate; $C_5H_{10}O_3$; [105-58-8]

Original Measurements:
O. de la Iglesia, A. M. Mainar, J. I. Pardo, and J. S. Urieta, J. Chem. Eng. Data **48**, 657–661 (2003).

Variables:
T/K = 298.15
p_1 /MPa = 0.10133

Prepared By:
H. L. Clever

Experimental Values

The solubility of tetrafluoromethane in four solvents at 298.15 K and a partial pressure of 0.10133 MPa

Solvent	$10^4 x_1$	Henry's Constant ($H_{1,2}$ /bar)	Ostwald Coefficient (L/cm^3 cm^{-3})
Tri(ethylene glycol) dimethyl ether	5.696	1766	0.0767
Tetra(ethylene glycol) dimethyl ether	5.215	1929	0.0578
Dimethyl carbonate	6.871	1464	0.1977
Diethylcarbonate	10.72	938.3	0.2166

The compiler calculated and added the Ostwald coefficients assuming ideal gas behavior.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. It was described in detail in an earlier paper of the authors.[1,2] The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements are carried out on the solvent saturated gas.

Source and Purity of Material:
(1) Tetrafluoromethane. Air Liquide. Stated to be 99.999%.
(2) Tri(ethylene glycol) dimethyl ether. Aldrich. 99 mol %. Density 980.2 kg m^{-3}; dipole moment 2.16 D.
(2) Tetra(ethylene glycol) dimethyl ether. Aldrich. 99 mol %. Density 1006.2 kg m^{-3}; dipole moment 2.44 D.
(2) Dimethyl carbonate. Fluka. 99 mol %. Density 1059.1 kg m^{-3}; dipole moment 0.86 D.
(2) Diethyl carbonate. Fluka. 99.5 mol %. Density 975.3 kg m^{-3}; dipole moment 0.86 D.

Estimated Error:
δT/K = ±0.05 cell; ±0.2 burets.
δp/kPa = ±3
$\delta x_1 / x_1$ = < ±0.01 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencieas Zaragoza **34**, 115–122 (1979).
[2]A. M. Mainar, J. Pardo, J. I. Garcia, F. M. Royo, and J. S. Urieta, J. Chem. Soc., Faraday Trans. **94**, 3595–3599 (1998).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [75-89-8]

Original Measurements:
(1) A. M. Mainar, J. Pardo, F. M. Royo, M. C. Lopez, and J. S. Urieta, J. Solution Chem. **25**, 589–595 (1996).
(2) M. A. Sanchez, A. M. Mainar, J. I. Pardo, M. C. Lopez, and J. S. Urieta, Can. J. Chem. **79**, 1460–1465 (2001).

Variables:
T/K = 268.15, 283.15, and 298.15
p_1 /kPa = 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
268.15	16.87	0.542	0.532
283.15	14.99	0.474	0.491
298.15	13.14	0.408	0.445

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction and density values using the solvent density in the paper and assuming ideal gas behavior. The 268.15 and 283.15 K values are from the 2001 paper and the 298.15 K value is from the 1996 paper.

The authors fit the data to the equation: $\ln x_1 = -8.827 + 655.867/(T/\mathrm{K})$, with $r^2 = 0.9981$.

Calculated from the equation: $\Delta H°$/kJ mol^{-1} = −5.452 and $\Delta S°$/J K^{-1} mol^{-1} = −73.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a five buret system, a pressure transducer system, and a solution vessel of 85 cm^3 for the CF_4 and of 27 cm^3 for the SF_6 . The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. To reduce the data from the working pressure to 101.33 kPa the following simplifications are assumed: (1) the liquid activity coefficients are assumed to be unity, (2) the fugacity coefficients can be obtained from a virial equation truncated after the second term, and (3) for the partial molar volumes in the Poynting correction the average values reported[3] were used for gases and the value calculated from the liquid density of the solvent was used for the solvent.

Source and Purity of Material:
(1) Tetrafluoromethane. J. T. Baker. Stated to be 99%.
(2) 2,2,2-Trifluoroethanol. Janssen Chimica. Purity stated to be 99%. Purity checked by GLC.

Estimated Error:
δT/K = ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.01 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza, **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).
[3]R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids* (McGraw Hill, New York, 1986).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) 1,1,1,3,3,3-Hexafluoropropan-2-ol; $C_3H_2F_6O$; [920-66-1]

Original Measurements:
(1) A. M. Mainar, J. Pardo, J. I. Garcia, F. M. Royo, and J. S. Urieta, J. Chem. Soc., Faraday Trans. **94**, 3595–3599 (1998).
(2) M. A. Sanchez, A. M. Mainar, J. A. Pardo, M. C. Lopez, and J. S. Urieta, Can. J. Chem. **79**, 1460–1465 (2001).

Variables:
T/K= 268.15, 283.15, and 298.15
p_1 /kPa= 101.32

Prepared By:
H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
268.15	38.76	0.861	0.845
283.15	35.57	0.774	0.802
298.15	32.15	0.690	0.753

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction and density values assuming ideal gas behavior. The 268.15 K and 283.15 K values are in the 2001 paper and the 298.15 K value is in the 1998 paper.
The authors fit the data to the equation: $\ln x_1 = -7.754 + 600.523/(T/\mathrm{K})$ with $r^2 = 0.9991$.
Calculated from the equation: $\Delta H°$/kJ mol^{-1} = −4.993 and $\Delta S°$/J K^{-1} mol^{-1} = −64.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to that of Ben-Naim and Baer. The authors have described their apparatus in earlier papers.[1,2] The apparatus consists of a five buret system, a pressure transducer system, and a solution vessel of 85 cm^3 for the CF_4 and of 27 cm^3 for the SF_6 . The solvent is degassed in the solution vessel. Measurements were carried out on solvent vapor saturated gas. To reduce the data from the working pressure to 101.33 kPa the following simplifications are assumed: (1) the liquid activity coefficients are assumed to be unity, (2) the fugacity coefficients can be obtained from a virial equation truncated after the second term, and (3) for the partial molar volumes in the Poynting correction the average values reported[3] were used for gases and the value calculated from the liquid density of the solvent was used for the solvent.

Source and Purity of Material:
(1)Tetrafluoromethane. J. T. Baker. Stated to be 99%.
(2) Hexafluoropropan-2-ol. Fluorchem Ltd. Purity stated to be >99%. Checked by GLC. At 298.15 K: Density 1604.23 kg m^{-3}. Vapor pressure 21.17 kPa from literature.

Estimated Error:
δT/K= ±0.05 cell; = ±0.2 burets.
$\delta x_1 / x_1$ = ±0.01 (authors).

References:
[1]J. Carniecer, F. Gibanel, J. S. Urieta, and C. Gutierrez Losa, Rev. Acad. Ciencias Zaragoza **34**, 115–122 (1979).
[2]M. A. Gallardo, J. S. Urieta, and C. Gutierrez Losa, J. Chim. Phys. **80**, 621 (1983).
[3]R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids* (McGraw Hill, New York, 1986).

Components:
(1) Tetrafluoromethane; CF_4 ; [75-73-0]
(2) Tetrachloromethane; CCl_4 ; [56-23-5]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K= 279.51–307.54
p_1 /kPa= 101.325

Prepared By:
H. L. Clever

Experimental Values

The solubility of CF_4 in tetrachloromethane at a partial pressure of 101.325 kPa between 279.51 K and 307.54 K

t/°C	T/K	$10^4/x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^{-3} cm^{-3})
6.36	279.51	11.91	0.282	0.289
14.56	287.71	11.36	0.266	0.280
24.48	297.63	11.91	0.275	0.300
34.39	307.54	11.99	0.274	0.308

The compiler calculated the Bunsen and Ostwald coefficient values assuming ideal gas behavior. Smoothed data, for use between 279.51 K and 307.54 K (the value at 287.71 K was omitted).
The smoothed data treatment yields: $\ln x_1 = -6.6711 - 0.1757/(T/100\ \mathrm{K})$.
The standard error about the regression line is 4.28×10^{-6}, and the smoothed data are:

T/K	$10^4 x_1$
278.15	11.89
288.15	11.92
298.15	11.94
308.15	11.97

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25 °C, the pipet at any temperature from 5 to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid nitrogen, then evacuating and then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements in the buret before and after introduction of gas into the pipet. The stirrer is set in motion Equilibration is attained within 24 h.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Minimum specified purity 95 mol %. Purified further by multiple trap distillations.
(2) Tetrachloromethane. Brothers Chemical Co. A. R. Grade. Refluxed over mercury, washed with 5 wt % NaOH and with water, dried over P_2O_5 and distilled.

Estimated Error:
$\delta x_1 / x_1$ = ±0.002 (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) 1,1,2,2,3,3,4,4,4-Nonafluoro-*N*,*N*-bis(nonafluorobutyl)-1-butanamine or perfluorotributylamine; $C_{12}F_{27}N$; [311-89-7]

Original Measurements:
R. J. Powell, J. Chem. Eng. Data **17**, 302–304 (1971).

Variables:
T/K = 288.15–318.15
p/kPa = 101.325

Prepared By:
P. L. Long and H. L. Clever

Experimental Values

T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})	Slope N [$R(\Delta \log x_1/\Delta \log T)$]
298.15	148.1	0.944	1.03	−5.35

The Bunsen and Ostwald coefficients were calculated by the compilers assuming ideal gas and Henry's law behavior. The author states that solubility measurements were made over the temperature interval of about 288.15–318.15 K. Only the solubility value of 298.15 K was given in the paper. The slope, $N = R(\Delta \log x_1/\Delta \log T)$ was given.

Smoothed Data for use between 288.15 K and 318.15 K was calculated by the compiler from the author's slope and solubility value at 298.15 K. The slope equation was rearranged by the compilers to

$$\lg x_1 = \lg(0.01481) - (5.35/R)\lg[(T/\mathrm{K})/298.15] \quad \text{with} \quad R = 1.9872 \text{ cal K}^{-1}\text{ mol}^{-1}.$$

T/K	x_1
288.15	0.01623
298.15	0.01481
308.15	0.01355
318.15	0.01355

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is the Diamond and Hildebrand[1] apparatus which uses an all glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final pressures. The solvent is degassed by freezing, pumping and followed by boiling under reduced pressure.

Source and Purity of Material:
(1) Tetrafluoromethane. Source not given. Stated to be manufacturer's research grade, dried over $CaCl_2$ before use.
(2) Perfluorotributylamine. Minnesota Mining and Manufacturing Co. Distilled, used portion boiling between 447.85–448.64 K which gave a single GLC peak. Density at 298.15 K, $\rho = 1.880$ g cm^{-3}.

Estimated Error:
$\delta x_1/x_1 = \pm 0.002$
δN/cal K^{-1} mol^{-1} = ±0.1

References:
[1]J. H. Diamond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Bromocyclohexane; $C_6H_{11}Br$; [108-85-0]

Original Measurements:
M. C. Lopez, M. A. Gallardo, J. S. Urieta, and C. Gutierrez, J. Chem. Eng. Data **32**, 472–474 (1989).

Variables:
T/K = 263.15–303.15
p_1/bar = 1.013

Prepared By:
C. L. Young

Experimental Values

T/K	$10^4 x_1$
263.15	3.88
273.15	4.01
283.15	4.12
293.15	4.23
303.15	4.33

The authors fitted the data to the equation: $\ln x_1 = -6.2045 + (252.3418/(T/\mathrm{K})) + 0.1237 \ln(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility apparatus was similar to that used by Ben-Naim and Baer[1] consisting essentially of a gas buret, mercury manometer, and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It was assumed that the mole fraction of the solvent was that corresponding to the vapor pressure of the pure solvent. It appears that the mole fraction at a partial pressure of 1 atm was estimated from raw experimental data assuming Henry's law is obeyed.

Source and Purity of Material:
(1) Tetrafluoromethane. J. T. Baker Co. Purity stated to be 99 mole %.
(2) Bromocyclohexane. Fluka. Purity 99+ mole % as determined by gas chromatography.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1 = \pm 0.015$

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]

Original Measurements:
M. C. Lopez, M. A. Gallardo, J. S. Urieta, and C. Gutierrez, J. Chem. Eng. Data **32**, 472–474 (1989).

Variables:
T/K = 263.15–303.15
p_1 /bar = 1.013

Prepared By:
C. L. Young

Experimental Values

T/K	$10^4 x_1$
263.15	5.88
273.15	5.93
283.15	5.98
293.15	6.05
303.15	6.13

The authors fitted the data to the equation: $\ln x_1 = -14.1898 + [217.8/(T/\mathrm{K})] + 1.0627 \ln(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility apparatus was similar to that used by Ben-Naim and Baer[1] consisting essentially of a gas buret, mercury manometer, and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It was assumed that the mole fraction of the solvent was that corresponding to the vapor pressure of the pure solvent. It appears that the mole fraction at a partial pressure of 1 atm was estimated from raw experimental data assuming Henry's law is obeyed.

Source and Purity of Material:
(1) Tetrafluoromethane. J. T. Baker Co. Purity stated to be 99 mole %.
(2) Chlorocyclohexane. Merck and Co. Purity stated to be 98.5 mole %, main impurity cyclohexane at 0.4 mole %.

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.015

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Chlorotrifluoromethane; $CClF_3$; [75-72-9]

Original Measurements:
P. C. Proust and F. P. Stein, J. Chem. Eng. Data **24**, 341–343 (1979).

Variables:
T/K = 199.80
p_{tot} /MPa = 0.1544–1.5272

Prepared By:
H. L. Clever

Experimental Values

T/K	Pressure* (P_{tot} /bar)	Liquid phase x_1	Vapor phase x_1
199.80	1.544	0.0000	0.0000
	2.013	0.0277	0.2278
	2.448	0.0540	0.3805
	3.447	0.1192	0.5811
	3.599	0.1248	0.6017
	5.323	0.2422	0.7534
	6.895	0.3617	0.8283
	8.487	0.4942	0.8772
	10.349	0.6489	0.9165
	12.031	0.7783	0.9479
	13.755	0.8949	0.9737
	15.272	1.0000	1.0000

*1 MPa = 10 bar.

Auxiliary Information

Method/Apparatus/Procedure:
A vapor re-circulation apparatus was used. Its description, construction, and mode of operation have been reported.[1,2]

Source and Purity of Material:
(1) Tetrafluoromethane. E. I. DuPont & Co. Stated purity of 99.7% confirmed by GLC. Major impurity is air.
(2) Chlorotrifluoromethane. E. I. DuPont & Co. Stated purity of 99.9% confirmed by GLC. Major impurity is CF_4.

Estimated Error:
δT/K = ±0.01
δp_{tot} /bar = ±0.007
$\delta x/x$ = ±0.003 for lesser x.

References:
[1]F. P. Stein, C. J. Sterner, and J. M. Geist, Chem. Eng. Prog. **58**, 70 (1962)
[2]F. P. Stein and P. C. Proust, J. Chem. Eng. Data **16**, 389 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Tetrachloromethane or carbon tetrachloride; CCl_4; [56-23-5]

Original Measurements:
T. Tominaga, R. Battino, B. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175–180 (1986).

Variables:
T/K = 298.14–318.11
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of CF_4 in CCl_4 at 101.325 kPa and 298.14–318.11 K

T/K	$10^4 x_1$	Ostwald Coefficient (L/cm^3 cm^{-3})	Henry's Constant (10^{-6}/Pa)
298.14	318.11	0.2871	87.85
308.15	11.59	0.2871	87.41
308.15	11.95	0.3037	84.79
318.11	11.51	0.2980	88.06

The compiler calculated the mole fractions from the author's Henry's constants with no corrections.
Henry's constant, H/Pa = (p_1 /Pa)/x_1 (101 325 Pa = 1 atm).
The authors smoothed their data with the following equations:

$$\ln[H_{1,2}(T,p_{s,2})]/\mathrm{Pa} = 18.3069 - 7.78/(T/\mathrm{K})$$

and

$$\ln[L_{1,2}(T,p)] = -6.3181 - 180.57/(T/\mathrm{K}).$$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Ben-Naim and Baer.[1] It allows no contact between Hg and CCl_4. The degassing apparatus is that described by Battino *et al.*[2]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and a vacuum intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm. Solubility Determination. The procedure of Ben-Naim and Baer is followed. The gas is solvent vapor saturated, dissolution is usually complete within 10–20 min. The mixing volume chamber volumes are 26, 65, 380, and 1650 cm^3 calibrated to $\pm$0.01 cm^3. The pressure is maintained constant and the volume changed by a microprocessor controlled stepping motor operating a piston in a precision bore tube.

Source and Purity of Materials:
(1) Tetrafluoromethane. Matheson and Co. Stated to be 99.7 mol % pure.
(2) Tetrachloromethane. Fisher "Certified" grade. Stated to be 99 mol % pure. Distilled through a 1.2 m packed column, middle 80% stored, protected from light until used.

Error Estimate:
$\delta T/K = \pm 0.0.1$
$\delta x_1 / x_1 = \pm 0.01$ (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2935 (1963).
[2]R. Battino, M. Banzhof, M. Brogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Hexafluorobenzene; C_6F_6; [392-56-5]

Original Measurements:
D. F. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753–760 (1971).

Variables:
T/K = 282.91–297.83
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
9.76	282.91	50.69	1.008	1.044
9.77	282.92	49.92	1.008	1.028
24.42	297.57	45.92	0.894	0.974
24.68	297.83	45.56	0.886	0.966

The compiler calculated the Bunsen coefficients, assuming an ideal gas and Henry's law behavior.
Smoothed data for use between 282.91 K and 298.15 K: $\ln x_1 = -7.2085 + 5.4213/(T/100\ \mathrm{K})$.
The standard error about the regression line is 4.09×10^{-5}.

T/K	$10^4 x_1$
283.15	50.22
288.15	48.58
293.15	47.05
298.15	45.61

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility determination. The degassed solvent is passed in a thin film down a glass helical tube containing the solute gas and solvent vapor pressure at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Tetrafluoromethane. Either Air Products and Chemicals Inc. or the Matheson Co., Inc. Purest grade available. Minimum purity 99.0 mole % (usually >99.9 mol %).
(2) Hexafluorobenzene. Imperial Smelting Co., Avnomouth, U. K. GC purity 99.7%, density, ρ/g cm^{-3} = 1.60596 at 298.15 K. Purification described Anal. Chem. **40**, 224 (1968).

Estimated Error:
δT/K = $\pm$0.03
δp/mmHg = $\pm$0.5
$\delta x_1 / x_1 = \pm 0.005$

References:
[1]T. J. Morrison and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and W. F. Danforth, J. Am. Oil Chem. Soc. **48**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Tetrafluoromethane; CF_4; [75-73-0]
(2) Carbon disulfide; CS_2; [75-15-0]

Original Measurements:
G. Archer and J. H. Hildebrand, J. Phys. Chem. **67**, 1830–1833 (1963).

Variables:
T/K=279.63–308.06
p_1/kPa=101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in carbon disulfide at a partial pressure of 101.325 kPa between 279.63 K and 308.06 K

t/°C	T/K	$10^4 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
6.48	279.63	1.81	0.0684	0.0700
14.74	287.89	1.89	0.0707	0.0745
24.37	297.52	2.09	0.0773	0.0842
34.91	308.06	2.13	0.0778	0.0877

The compiler calculated the Bunsen and Ostwald coefficient values assuming ideal gas behavior.
Smoothed data for use between 278.15 K and 308.15 K: $\ln x_1 = -6.8370 - 4.9864(T/100\ \mathrm{K})$.
The value at 297.52 K was omitted from the smoothed data treatment.
The standard error about the regression line is 1.11×10^{-6}.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus[1] consists of a gas measuring buret, an absorption pipet and a reservoir for the solvent. The buret is thermostated at 25 °C, the pipet at any temperature from 5 °C to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid nitrogen, then evacuating and then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by p-V measurements in the buret before and after introduction of gas into the pipet. The stirrer is set in motion. Equilibration is attained within 24 h.

Source and Purity of Material:
(1) Tetrafluoromethane. Matheson Co., Inc. Minimum specified purity 95 mol %. Purified further by multiple trap distillations.
(2) Carbon disulfide. Brothers Chemical Co. Analytical Reagent Grade. Distilled from lime, treated with $KMnO_4$ solution, separated, shaken with mercury, and then with mercuric sulfate, dried over P_2O_5 and distilled. Stored over mercury.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.01$ (authors).

References:
[1]Y. Kobatake and J. H. Hildebrand, J. Phys. Chem. **65**, 331 (1961).

3.6. Trifluormethane

Components:
(1) Trifluoromethane; CHF_3; [75-46-7]
(2) Water; H_2O; [7732-16-5]

Evaluators:
H. Lawrence Clever,
Emory University,
Atlanta, GA 30322
September 2002.

Evaluation

In addition to the trifluoromethane+water system there are some comments on the trifluoromethane+sodium chloride +water system.

Trifluoromethane+Water

Three laboratories report solubility data on the CHF_3+H_2O system. Parmelee[1] shows most of his results in graphs; Wilhelm *et al.*[2] analyzed the data and give an equation for the mole fraction solubility at 1 atm between 298 K and 348 K. Zheng *et al.*[3] made measurements below atmospheric pressure at three temperatures near 278, 308, and 338 K. They also report measurements in three concentrations of aqueous NaCl at the same temperatures. Alexander *et al.*[4] made 16 measurements between 288 K and 303 K. Unfortunately the agreement among the laboratories is poor. The mole fraction solubility at 298.15 K and 1 atm partial pressure CHF_3 from the three is:

$10^4 x_1$	Reference
2.43	1, 2
1.74	3
3.75	4

The average and standard deviation are 2.64± 1.02. The deviation is 39% of the average value, which is unacceptable. To the best of our knowledge all of the laboratories have the reputation of doing careful and reliable work. There is no good reason to pick one set of values over another. Thus the results are classed as doubtful, use with caution. The problem will be resolved only with new experimental studies.

Trifluoromethane+Sodium chloride+Water

Zheng *et al.*[3] report the solubility of CHF_3 in water and in 0.0121, 0.0295, and 0.0564 mol NaCl per mole of water solutions at temperatures of 278, 308, and 338 K and pressures between 0.069 and 0.095 MPa. The corresponding NaCl molalities are 0.672, 1.64, and 3.13 mol kg^{-1}. The largest molality is near saturation. Both Zheng and Knapp have the reputation of careful and reliable workers, but the questions about the water solubility values above make us recommend caution in the use of these data. The Sechenow salt effect parameter in NaCl molality and CHF_3 mole fraction were calculated by the evaluator with the following results:

T/K	NaCl/mol kg-1 (three molalities studied)	Salt effect parameters, k_{smx}/kg mol^{-1} corresponding to the three molalities given at the left
278	$m_1=0.67$, $m_2=1.64$, $m_3=3.13$	$k_1=0.082$, $k_2=0.088$, $k_3=0.097$
308	$m_1=0.67$, $m_2=1.64$, $m_3=3.13$	$k_1=0.073$, $k_2=0.086$, $k_3=0.107$
338	$m_1=0.67$, $m_2=1.64$, $m_3=3.13$	$k_1=0.083$, $k_2=0.097$, $k_3=0.131$

The magnitude of the salt effect parameter is in the range often observed for other gases in aqueous NaCl, however there usually is a definite decrease in the salt effect parameter with increase in temperature that is not apparent here. The values are about the right order of magnitude, but scattered, use with caution.

References
[1]H. M. Parmelee, Refrig. Eng. **61**, 1341–1345 (1953).
[2]E. Wilhelm, R. Battino, and W. J. Wilcock, Chem. Rev. **77**, 219 (1977).
[3]D.-Q. Zheng, T.-M. Guo, and H. Knapp, Fluid Phase Equil. **129**, 197–209 (1997).
[4]A. F. M. Alexander, A. G. M. Abel, and I. M. A. Fonseca, Fluid Phase Equil. **173**, 97–107 (2000).

Components:
(1) Trifluoromethane; CHF_3; [75-46-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. M. Parmelee, Refrig. Eng. **61**, 1341–1345 (1953).

Variables:
T/K = 298.2, 323.2, and 348.2
p_1 /kPa = to ~ 2350

Prepared By:
H. L. Clever

Experimental Values

Solubility of tetrafluoromethane in water at 25 °C (298.2 K) at 101.3, 344.6, and 689.1 kPa

p_1 /psia	p_1 /kPa	s_1 /lb gal^{-1}	c_1 /mol L^{-1}	$10^5 x_1$
14.7	101.3	0.008	0.014	25
50	344.6	0.027	0.046	83
100	344.6	0.027	0.085	154

The compiler estimated the concentration and mole fraction solubility values assuming ideal gas behavior and Henry's law. Only the above values were tabulated. Other values were shown graphically in Figs. 3 and 9 of the original paper. Isotherms at 77, 122, and 167 °F were shown at pressures up to 340 psia (pounds per square inch absolute) were shown in Figs. 5 and 11 of the original paper.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus consisted of two parts. The first part a steel saturating cylinder for saturations above 1 atm, the second part a conical glass flask, buret, and manometer system.
Gas and water were contacted in the steel cylinder. They were stirred vigorously for 5 h. The line was purged and a saturated sample was transferred to the evacuated conical flask and buret and manometer system for measurement of the gas volume and the water weight.
At atmospheric pressure the water was saturated directly in the low pressure side of the system.

Source and Purity of Material:
(1) Trifluoromethane or Freon-23. DuPont Co. product.
(2) Water. Distilled.

Estimated Error:
δt/°F = ± 0.2
$\delta s_1 / s_1$ = ± 0.05
Gas volumes measured to ± 0.1 mL;
Water weighed to ± 0.1 g.

Components:
(1) Trifluoromethane; CHF_3; [75-46-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. F. M. Alexander, A. G. M. Abel, and I. M. A. Fonseca, Fluid Phase Eq. **173**, 97–107 (2000).

Variables:
T/K = 288.30–303.03
p_1 /Pa = 101325

Prepared By:
H. L. Clever

Experimental Values

Solubility of trifluoromethane in water from 288.03 K to 303.03 K. Mole fraction and Ostwald coefficients at a pressure of 101 325 Pa

T/K	$10^4 x_1$	Ostwald Coefficient ($L_{1,2}$ /cm^3 cm^{-3})	Henry's Constant (H_1 /MPa)
288.03	5.067	0.660	200.0
290.55	4.800	0.630	211.1
291.55	4.685	0.617	216.3
292.30	4.608	0.608	219.9
293.15	4.437	0.587	228.4
293.67	4.367	0.579	232.0
294.30	4.308	0.572	235.2
295.25	4.157	0.554	243.8
296.00	4.089	0.546	247.8
297.08	3.961	0.531	255.8
297.60	3.891	0.522	260.4
298.38	3.823	0.514	265.0
299.68	3.681	0.497	275.3
300.50	3.596	0.487	281.8
301.49	3.485	0.473	290.7
303.03	3.377	0.461	300.2

The authors fitted the mole fraction solubility to the equation: $R \ln x_1 = -135.348 + 20{,}860.7/(T/\mathrm{K})$ from which they obtained ΔH/J mol^{-1} = −20 861 and ΔS/J K^{-1} mol^{-1} = −135.35.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and technique were given in detail in Silva *et al.*[1] See methyl fluoride + alcohol data sheets earlier in this volume. The principle of the method is to bring a measured volume of degassed water into contact with a known volume of gas at a given temperature and pressure. After equilibrium is attained the change in volume gives the amount of gas dissolved and the solubility.
The method was tested by measuring the solubilities of oxygen and of carbon dioxide in water. The results agreed with literature values to ± 2%.

Source and Purity of Material:
(1) Trifluoromethane or HFC-23. Linde Gas. Purity stated to be 99.9 mol %.
(2) Water. Purified. Degassed by vacuum sublimation technique.

Estimated Error:
δT/K = ± 0.01
δp/mmHg = ± 0.01
$\delta x_1 / x_1$ = ± 0.02

References:
[1]C. S. O. Silva, I. M. A. Fonseca, and L. Q. Lobo, Fluid Phase Eq. **135**, 137 (1997).

Components:
(1) Trifluoromethane; CHF_3; [75-46-7]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
D.-Q. Zheng, T.-M. Guo, and H. Knapp, Fluid Phase Eq. **129**, 197–209 (1997).

Variables:
T/K = 278.13–338.21
p/MPa = 0.06875–0.09466

Prepared By:
H. L. Clever

Experimental Values

Solubility of CHF_3 in water and aqueous NaCl

T/K	p/MPa	NaCl (n_2/mol mol^{-1})	CHF_3 ($10^4 x_1$)	Henry's Constant ($H_{1,s}$/MPa)
278.20	0.06875	0.00	2.87	235.1
278.20	0.06916	0.00	2.90	234.1
308.15	0.08133	0.00	1.34	560.9
308.15	0.08248	0.00	1.36	561.4
338.21	0.09005	0.00	0.705	915.9
338.21	0.09147	0.00	0.712	925.6
278.15	0.06926	0.0121	2.56	266.1
278.15	0.07084	0.0121	2.61	266.9
308.09	0.08159	0.0121	1.21	626.1
308.09	0.08366	0.0121	1.23	629.9
338.17	0.09043	0.0121	0.627	1041
338.17	0.09224	0.0121	0.637	1052
278.15	0.06988	0.0295	2.10	326.4
278.15	0.07242	0.0295	2.17	327.4
308.09	0.08021	0.0295	0.96	772.7
308.09	0.08358	0.0295	1.00	779.1
338.14	0.08847	0.0295	0.486	1311
338.14	0.09146	0.0295	0.496	1311
278.13	0.07787	0.0564	1.61	477.5
278.13	0.07825	0.0564	1.63	468.6
308.06	0.08656	0.0564	0.671	1221
308.06	0.08770	0.0564	0.672	1202
338.13	0.09357	0.0564	0.293	2375
338.13	0.09466	0.0564	0.298	2372

The above NaCl mol ratios correspond to 0.672, 1.64, and 3.13 mol kg^{-1} (molality), respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental apparatus consists of a degassing system and a gas absorption unit. The water and NaCl solutions were degassed by vacuum with stirring until the vapor pressure of the solvent was reached. The degassed solvent was transferred to an evacuated glass cell and weighed to 0.0001 g. The cell was thermostated and the adsorption apparatus evacuated before the gas was admitted. The solvent was stirred constantly. When the system T and p were constant, the equilibrium state was established.

Source and Purity of Material:
(1) Trifluoromethane or R-23. Hoechst. Purity stated to be 99.0 volume %.
(2) Sodium chloride. Merck. Laboratory grade.
(3) Water. Deionized at the Institute.

Estimated Error:
δT/K = ±0.1
$\delta p/p$ = ±0.001
$\delta x_1/x_1$ = ±0.005
Compiler's estimates.

Components:
(1) Trifluoromethane or HFC-23; CHF_3; [75-46-7]
(2) 1,1-Difluoroethane or HFC-152a; $C_2H_4F_2$; [75-37-6]

Original Measurements:
J. S. Lim, K. H. Park, and B. G. Lee, J. Chem. Eng. Data **47**, 582–586 (2002).

Variables:
T/K = 283.15, 293.15
p_{exp}/MPa = 0.374–4.203

Prepared By:
H. L. Clever

Experimental Values

Vapor liquid equilibrium in the $CHF_3 + C_2H_4F_2$ system at 283.15 K and 293.15 K

T/K	p_{exp}/MPa	Liquid phase x_1	Vapor phase x_1
283.15	0.374	0.000	0.000
283.15	0.427	0.024	0.111
283.15	0.540	0.082	0.321
283.15	0.632	0.124	0.430
283.15	0.867	0.230	0.598
283.15	1.249	0.384	0.749
283.15	1.667	0.525	0.838
283.15	2.330	0.754	0.931
283.15	2.695	0.851	0.960
283.15	3.275	1.000	1.000
293.15	0.515	0.000	0.000
293.15	0.618	0.045	0.173
293.15	0.728	0.083	0.297
293.15	0.890	0.140	0.434
293.15	1.195	0.244	0.597
293.15	1.570	0.377	0.726
293.15	2.106	0.550	0.835
293.15	2.505	0.654	0.882
293.15	3.379	0.851	0.952
293.15	4.203	1.000	1.000

Auxiliary Information

Method/Apparatus/Procedure:
A circulation type apparatus was used in which both vapor and liquid phases were continuously circulated. The 85 cm^3 316 stainless steel equilibration vessel was equipped with a pair of Pyrex glass windows. Stirring was by a variable rate magnetic stirrer. At equilibrium stirring was stopped, pressure measured, vapor and liquid samples were withdrawn from the recycling loop and injected into a gas chromatograph equipped with a thermal conductivity detector

Source and Purity of Material:
(1) HFC-23. DuPont Co. Guaranteed purity of 99.9 mass %. Used as received.
(2) HFC-152a. DuPont Co. Guaranteed purity of 99.9 mass %. Used as received.

Estimated Error:
δT/K = ±0.05
δp/kPa = ±5
Composition = ±0.2 mole %.

Components:
(1) Trifluoromethane or HFC-23; CHF_3; [75-46-7]
(2) 1,1,1-Trifluoroethane or HFC-143a; $C_2H_3F_3$; [420-46-2]

Original Measurements:
J. S. Lim, K. H. Park, and B. G. Lee, J. Chem. Eng. Data **47**, 582–586 (2002).

Variables:
T/K = 283.15 and 293.15
p_{exp} /MPa = 0.838–4.203

Prepared By:
H. L. Clever

Experimental Values

Vapor liquid equilibrium in the $CHF_3 + C_2H_3F_3$ system at 283.15 K and 293.15 K

T/K	p_{exp} /MPa	Liquid phase x_1	Vapor phase x_1
283.15	0.838	0.000	0.000
283.15	0.968	0.070	0.165
283.15	1.108	0.146	0.298
283.15	1.341	0.255	0.466
283.15	1.593	0.375	0.595
283.15	1.862	0.485	0.699
283.15	2.106	0.580	0.771
283.15	2.385	0.690	0.839
283.15	2.655	0.784	0.892
283.15	3.275	1.000	1.000
293.15	1.104	0.000	0.000
293.15	1.331	0.103	0.214
293.15	1.506	0.178	0.335
293.15	1.801	0.296	0.491
293.15	2.100	0.402	0.606
293.15	2.522	0.550	0.727
293.15	2.909	0.664	0.806
293.15	3.286	0.759	0.866
293.15	3.804	0.898	0.942
293.15	4.203	1.000	1.000

Auxiliary Information

Method/Apparatus/Procedure:
A circulation type apparatus was used in which both vapor and liquid phases were continuously circulated. The 85 cm^3 316 stainless steel equilibration vessel was equipped with a pair of Pyrex glass windows. Stirring was by a variable rate magnetic stirrer. At equilibrium the stirring was stopped, pressure measured, vapor and liquid samples withdrawn from the recycling loop and injected into a gas chromatograph equipped with a thermal conductivity detector.

Source and Purity of Material:
(1) HFC-23. DuPont. Guaranteed purity of 99.9 mass %. Used as received.
(2) HFC-143a. DuPont. Guaranteed purity 99.9 mass %. Used as received.

Estimated Error:
δT/K = ±0.05
δp/kPa = ±5
Composition = ±0.2 mol %.

3.7. Difluoromethane

Components:
(1) Difluoromethane; CH_2F_2; [75-10-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. F. M. Alexander, A. G. M. Abel, and I. M. A. Fonseca, Fluid Phase Equil. **173**, 97–107 (2000).

Variables:
T/K = 289.16–302.26
p_1 /Pa = 101325

Prepared By:
H. L. Clever

Experimental Values

The solubility of difluoromethane in water from 289.16 K to 302.26 K. Mole fraction and Ostwald coefficients at a pressure of 101 325 Pa

T/K	$10^4 x_1$	Ostwald Coefficient ($L_{1,2}$ /cm^3 cm^{-3})	Henry's Constant (H_1 /MPa)
289.16	7.584	0.985	133.6
290.50	7.305	0.953	138.7
291.29	7.107	0.930	142.6
292.35	6.898	0.906	146.9
293.14	6.743	0.888	150.3
294.20	6.407	0.847	158.1
294.99	6.238	0.827	162.4
296.04	5.998	0.798	168.9
297.08	5.689	0.759	178.1
298.12	5.452	0.730	185.9
298.90	5.358	0.719	189.1
299.94	5.049	0.680	200.7
301.23	4.743	0.641	213.6
302.26	4.469	0.606	226.7

The authors fitted the mole fraction solubility to the equation: $R \ln x_1 = -160.480 + 29\,204.5/(T/\mathrm{K})$ from which they obtained ΔH/J mol^{-1} = −29 205 and ΔS/J K^{-1} mol^{-1} = −160.48. (Reversed values in paper's Table 5.)

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and technique were given in detail in Silva *et al.*[1] See methyl fluoride+alcohol data sheets earlier in this volume. The principle of the method is to bring a measured volume of degassed water into contact with a known volume of gas at a given temperature and pressure. After equilibrium is attained the change in volume gives the amount of gas dissolved and the solubility.
The method was tested by measuring the solubilities of oxygen and of carbon dioxide in water. The results agreed with literature values to ±2%.

Source and Purity of Material:
(1) Difluoromethane or HFC-32. Linde Gas. Purity stated to be 99.9 mol %.
(2) Water. Purified. Degassed by vacuum sublimation technique.

Estimated Error:
δT/K = ±0.01
δp/mmHg = ±0.01
$\delta x_1 / x_1$ = ±0.02

References:
[1]C. S. O. Silva, I. M. A. Fonseca, and L. Q. Lobo, Fluid Phase Equil. **135**, 137 (1997).

Components:
(1) Difluoromethane; CH_2F_2; [75-10-5]
(2) Saline
(2) Olive oil
(2) Rat blood and tissues

Original Measurements:
M. L. Gargas, P. G. Seybold, and M. E. Anderson, Toxicol. Lett. **43**, 235–256 (1988).

Variables:
T/K = 310.15
p_1 /Pa is small and unknown.

Prepared By:
H. L. Clever

Experimental Values

Partition coefficients at 37 °C (310.15 K)

Solvent	Partition Coefficient $p_i = (c_{1\,\mathrm{liq}})/(c_{1\,\mathrm{gas}})$	Number of Determinations N
Saline	1.31 ± 0.05	4
Olive oil	4.76 ± 0.75	3
Blood	1.60 ± 0.10	4
Liver	2.75 ± 0.39	3
Muscle	1.44 ± 0.25	3
Fat	1.43 ± 0.31	4

All values are mean ± standard error of the mean. These data were published earlier.[2] The number of determinations and information on source and purity were taken from Ref. 2.

Auxiliary Information

Method/Apparatus/Procedure:
The saline (0.9%):air, olive oil:air, blood:air, and rat tissue:air partition coefficients, P_i, were determined at 37 °C by a vial equilibration proceedure.[1,2] The saline, oil, and blood were measured into the vial by volume. The tissues were homogenized in a 1:3 (weight tissue:volume saline) ratio using the 0.9 wt % saline. The calculation of the tissue partition coefficient was corrected for the solute gas in the saline. A sample of known volume is added to one vial, another vial of the same volume is kept empty. About 0.1 mL of a dilute solution of liquid halocarbon in water is added to each vial. Liquid-air equilibration is established by shaking the vial about 2 h in a 37 °C thermostat. A known volume, about 1 mL, is removed from test and reference vials, and analyzed for the halocarbon by GLC.

Source and Purity of Material:
(1) Difluormethane. Columbia Organic Chemical Co. The CH_2F_2 could be obtained only as a mixture with CH_2ClF. The partition coefficients were determined using the mixture of 30% CH_2F_2 and 70% CH_2ClF.
(2) Rat blood and tissues. Male Fisher-344 rats.

Estimated Error:
Temp.: Nothing specified.
Solubility: See standard errors in table above.

References:
[1]S. Sato and T. Nakajima, Br. J. Ind. Med. **36**, 231–234 (1979).
[2]M. L. Gargas, H. J. Clewell III, and M. E. Anderson, Toxicol. App. Pharacol. **82**, 211–223 (1986).

Components:
(1) 1,1-Difluoroethane or HFC-152a; $C_2H_4F_2$; [75-38-7]
(2) Tetracosane; $C_{24}H_{50}$; [646-31-1]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 551–561 (1997).

Variables:
T/K = 333.15 and 353.15

Prepared By:
H. L. Clever

Experimental Values

T/K	Henry's Constant (H/MPa)	Activity Coefficient γ
333.15	2.91	2.44
353.15	4.04	2.36

Auxiliary Information

Method/Apparatus/Procedure:
These values were measured about 1991 by a GLC method when the authors were at another laboratory.
These data are in Appendix A of the paper.

Source and Purity of Material:
(1) 1,2-Difluoroethane. Nothing specified.
(2) Tetracosane. Nothing specified.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.05$ authors.

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.14–313.06
p_t/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Temperature (T/K)	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant [$H_{1,2}$/MPa = (p_1/Mpa)/x_1]
283.14	0.0261	0.931	3.61
292.91	0.0169	0.8754	4.52
303.22	0.0148	0.7833	5.34
313.06	0.0099	0.6551	6.7

The authors approximated the difluoromethane partial pressure as: $p_1/\mathrm{MPa} = (p_t/\mathrm{MPa})y_1 = 0.1013y_1$.

They fitted the Henry's constants to the equation:

$$\ln(H_{1,2}/\mathrm{MPa}) = -70.077 + 1663.16/(T/\mathrm{K}) + 11.6\ln(T/\mathrm{K}).$$

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions.
Measurements were repeated three times.

Source and Purity of Material:
(1) Difluoromethane. Showa Denko. Stated to be 99.9% pure.
(2) Methanol. Wake Pure Chemicals, Ltd. Stated to be 99.8% pure.

Estimated Error:
$\delta T/\mathrm{K} = \pm 0.1$
$\delta x_1/x_1 = < \pm 0.02$ for the liquid phase
$= \pm 0.005$ for the vapor phase.
$\delta H/H = \pm 0.025$.

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
R. Kato and H. Nishiumi, J. Chem. Eng. Data **47**, 1140–1144 (2002).

Variables:
T/K = 303.0, 318.0, and 323.0
p/kPa = 56.2–111.0

Prepared By:
H. L. Clever

Experimental Values

The solubility of difluoromethane in methanol from 303.0 K to 323.0 K

T/K	p/kPa	Liquid Mol Fraction x_1	Vapor Mol Fraction y_1	Henry's Constant (H/MPa)
303.0	56.2	0.00700	0.582	4.64
	56.1	0.00700	0.575	
318.0	95.3	0.00720	0.516	6.93
	95.0	0.00700	0.511	
	91.3	0.00630	0.488	
323.0	111.0	0.00700	0.495	7.88
	99.4	0.00560	0.446	

The authors fit the Henry constants to the equation:

$$\ln(H/\mathrm{MPa}) = 33.19 - 3665/(T/\mathrm{K}) - 3.425\ln(T/\mathrm{K}).$$

At 303 K and 101 kPa, the mole fraction of CH_2F_2 in methanol is 0.0219 and the entropy of solution is $-69.17\ \mathrm{J\ K^{-1}\ mol^{-1}}$.

Auxiliary Information

Method/Apparatus/Procedure:
The method was head space gas chromatography. The HS-40 Perkin-Elmer head space autosampler as chromatograph was used. Equilibrium cells were 22 mL glass vials. The autosampler, in a constant temperature bath, could contain up to 13 vials. The solvent was weighed in a glass ampule and placed in a sample vial; the fluorocarbon was charged into the vial and weighed. The fluorocarbon weight and the air weight replaced by fluorocarbon were used to determine the overall composition. The solvent ampule was broken and the system equilibrated for 3 h, the headspace vapor was injected for 3 s into the gas chromatograph by the auto-sampler program. Details of the calculation are in the paper.

Source and Purity of Material:
(1) Difluoromethane. Toei Chem. Ind. (Tokyo). Purity stated to be 99.9%, used as received.
(2) Methanol. Kanto Chem. Ind. (Tokyo). Purity stated to be 99.5%, used as received

Estimated Error:
$\delta T/\mathrm{K} = \pm 0.1$
$\delta x_1/x_1 = \pm 0.008$ av.; ± 0.022 max.
$\delta y_1/y_1 = \pm 0.008$ av.; ± 0.021 max.

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.17–312.95
p_t/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant $[H_{1,2}/\text{MPa} = (p_1/\text{MPa})/x_1]$
283.17	0.0278	0.9735	3.54
292.96	0.0214	0.9518	4.50
303.81	0.0174	0.9099	5.30
312.95	0.0134	0.8448	6.40

The authors approximated the difluoromethane partial pressure as

$$p_1/\text{MPa} = (p_t/\text{MPa})y_1 = 0.1013y_1 .$$

They fitted the Henry's constants to the equation:

$$\ln(H_{1,2}/\text{MPa}) = 106.501 - 6132.004(T/\text{K}) - 14.802 \ln(T/\text{K}).$$

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions.
Measurements were repeated three times.

Source and Purity of Material:
(1) Difluoromethane. Showa Denko. Stated to be 99.9% pure.
(2) Ethanol. Wake Pure Chemicals, Ltd. Stated to be 99.8% pure.

Estimated Error:
δT/K = ± 0.1
$\delta x_1/x_1$ = < ± 0.02 for the liquid phase
= ± 0.005 for the vapor phase.
$\delta H/H = \pm 0.025$.

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
R. Kato and H. Nishiumi, J. Chem. Eng. Data **47**, 1140–1144 (2002).

Variables:
T/K = 303.0–323.0
p/kPa = 51.4–102.0

Prepared By:
H. L. Clever

Experimental Values

The solubility of difluoromethane in ethanol from 303.0 K to 323.0 K

T/K	p/kPa	Liquid Mol Fraction x_1	Vapor Mol Fraction y_1	Henry's Constant (H/MPa)
303.0	59.7	0.01010	0.798	4.66
	51.4	0.00880	0.782	
	53.3	0.00900	0.788	
308.0	70.7	0.00960	0.776	5.76
	72.3	0.00960	0.778	
	63.0	0.00820	0.755	
	63.2	0.00850	0.758	
313.0	78.6	0.00880	0.731	6.53
318.0	94.4	0.00840	0.716	8.13
	80.6	0.00660	0.677	
323.0	102.0	0.00720	0.682	9.62
	94.7	0.00650	0.655	

The authors fit the Henry constants to the equation $\ln(H/\text{MPa}) = 34.23 - 4497/(T/\text{K}) - 3.125 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
The method was head space gas chromatography. The HS-40 Perkin-Elmer head space autosampler gas chromatograph was used. Equilibrium cells were 22 mL glass vials. The autosampler, in a constant temperature bath, could contain up to 13 vials. The solvent was weighed in a glass ampule and placed in a sample vial; the fluorocarbon was charged into the vial and weighed. The fluorocarbon weight and the air weight replaced by fluorocarbon were used to determine the overall composition. The solvent ampule was broken and the system equilibrated for 3 h, the headspace vapor was injected for 3 s into the gas chromatograph by the auto-sampler program. Details of the calculation are in the paper.

Source and Purity of Material:
(1) Difluoromethane. Toei Chem. Ind. (Tokyo). Purity stated to be 99.9%, used as received.
(2) Ethanol. Kanto Chem. Ind. (Tokyo). Purity stated to be 99.5%, used as received

Estimated Error:
δT/K = ± 0.1
$\delta x_1/x_1 = \pm 0.008$ av.; ± 0.022 max.
$\delta y_1/y_1 = \pm 0.008$ av.; ± 0.021 max.

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) 2-Propanol; C_3H_8O; [67-63-0]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.16–313.18
p_t /MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant $[H_{1,2}$ /MPa $= (p_1$ /MPa$)/x_1]$
283.16	0.0210	0.9745	4.60
292.99	0.0174	0.9544	5.55
303.25	0.0143	0.9232	6.54
313,18	0.0116	0.8656	7.58

The authors approximated the difluoromethane partial pressure as p_1 /MPa $= (p_t$ /MPa$)y_1 = 0.1013y_1$.
They fitted the Henry's constants to the equation: $\ln(H_{1,2}$ /MPa$) = 3.88 - 1292.48(T/\mathrm{K}) + 0.396 \ln(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions.
Measurements were repeated three times.

Source and Purity of Material:
(1) Difluoromethane. Showa Denko. Stated to be 99.9% pure.
(2) 2-Propanol. Wake Pure Chemicals, Ltd. Stated to be 99.5% pure.

Estimated Error:
δT/K = ± 0.1
$\delta x_1 / x_1 = < \pm 0.02$ for the liquid phase
$= \pm 0.005$ for the vapor phase.
$\delta H/H = \pm 0.025$.

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) Pentaerythitol tetrapentanonate ester; $C_{25}H_{44}O_8$; [15834-04-5] *Chem. Abstr.* name: Pentanoic 2,2-*bis*[(1-oxypentyl)oxylmethyl]-1,3-propanediyl ester.

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823–828 (1999).

Variables:
T/K = 303.15–363.15
p_1 /MPa = 0.05–1.9

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1 MPa	Mol Fraction x_1
303.17	0.0711	0.0734	343.18	0.1072	0.0523
303.13	0.0937	0.0955	343.12	0.1415	0.0690
303.15	0.1238	0.1216	343.10	0.1844	0.0894
303.16	0.4078	0.3307	343.17	0.6253	0.2547
303.16	0.5830	0.4290	343.14	0.8948	0.3373
303.15	0.7947	0.5243	343.11	1.2485	0.4304
303.15	1.0738	0.6335	343.15	1.6178	0.5041
323.28	0.0903	0.0620	363.22	0.1226	0.0440
323.24	0.1189	0.0812	363.20	0.1612	0.0588
323.27	0.1560	0.1042	363.34	0.2095	0.0769
323.29	0.5237	0.2911	363.23	0.7140	0.2227
323.26	0.7510	0.3814	363.24	1.0153	0.2993
323.27	1.0375	0.4770	363.36	1.4276	0.3884
323.27	1.3827	0.5687	363.25	1.7949	0.4461

Henry's constant was calculated for the 12 points at pressures below 0.21 MPa and fitted to the equation
$\ln(\mathrm{He}_{1,2}$ /MPa$) = \ln(1.710 \pm 0.016) - (1873 \pm 47)[1/(T/\mathrm{K}) - 1/333.15]$.
The CH_2F_2 activity coefficients at infinite dilution are: $(T/\mathrm{K})/\gamma^{\infty}$ 303.2/0.67; 323.2/0.68; 343.2/0.71.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from pressure changes in a gas system of known volume, observed during the absorption of the gas. The apparatus consists of three sections. (i) A liquid bath thermostat 1 containing the equilibrium cell with a magnetic stirrer; (ii) liquid bath thermostat 2 with a gas bottle of calibrated volume; (iii) an air bath thermostat with a pressure transmitter and connections between the first two sections and to a gas storage and a vacuum pump. More details of the apparatus, the experimental technique, and the treatment of the data are in Wahlström and Vamling.[1]

Source and Purity of Material:
(1) Difluoromethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Pentaerythritol tetrapentanonate ester.
Synthesized[2] by a reaction between valeric acid and pentaerythirtol catalyzed with p-toluenesulfonic acid in a p-xylene solvent. The product was vacuum distilled. NMR and IR results gave a purity >95%.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p_1 / p_1 = \pm 0.001$
δHe/He = $< \pm 0.02$ at low pressures,
$= < \pm 0.03$ at high pressures.

References:
[1] Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2] K. D. Black and F. D. Gunstone, Chem. Phys. Lipids **56**, 169 (1990).

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) Pentaerythritol tetra-2-ethylhexanoate; $C_{37}H_{68}O_8$; [7299-99-2]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 303.10–363.25
p_1 /MPa = 0.1346–1.7624

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mole Fraction x_1	T/K	p_1 /MPa	Mole Fraction x_1
303.16	0.1346	0.1305	343.26	0.1818	0.0922
303.10	0.1466	0.1426	343.21	0.2001	0.0997
303.17	0.1551	0.1510	343.27	0.2112	0.1069
303.14	0.3901	0.3292	343.13	0.5588	0.2424
303.12	0.5202	0.3951	343.14	0.7593	0.3043
303.12	0.7677	0.5157	343.12	1.1742	0.4224
303.16	1.1357	0.6416	343.16	1.6146	0.5120
323.10	0.1590	0.1105	363.20	0.2005	0.0779
323.03	0.1748	0.1198	363.20	0.2207	0.0840
323.11	0.1847	0.1276	363.21	0.2332	0.0904
323.24	0.4827	0.2828	363.23	0.6214	0.2090
323.22	0.6488	0.3477	363.23	0.8490	0.2695
323.22	0.9870	0.4679	363.21	1.3344	0.3822
323.27	1.4121	0.5755	363.25	1.7624	0.4586

$$\ln(H_{2,1}/\text{MPa}) = \ln(1.666 \pm 0.008) - (1701 \pm 25)[1/(T/\text{K}) - 1/333.15]$$

Solvent Chem. Abstracts Name: 2,2-bis[(2-ethyl-1-oxohexyl)oxylmethyl]-1,3-propanediyl ester of 2-ethyl hexanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in Wahlström and Vamling.[1] The calculations of absorbed gas, Henry's constant, and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) Difluoromethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylhexanoate. Synthesized from pentaerythriiol and 2-ethyl-hexanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >90%. Contains 5%–10% di- and tri- esters.

Estimated Error:
Uncertanties in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) Pentaerythritol tetrananoate; $C_{41}H_{76}O_8$; [14450-05-6]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 303.09–363.23
p_1 /MPa = 0.2033–1.9372

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mole Fraction x_1	T/K	p_1 /MPa	Mole Fraction x_1
303.13	0.2033	0.1877	343.24	0.2525	0.1264
303.14	0.2174	0.1973	343.24	0.2702	0.1324
303.09	0.2339	0.2097	343.20	0.2904	0.1417
303.18	0.3783	0.2988	343.25	0.5197	0.2236
303.19	0.7137	0.4635	343.25	0.9458	0.3485
303.15	0.8820	0.5314	343.21	1.2496	0.4244
303.15	1.2908	0.6622	343.21	1.7887	0.5343
323.07	0.2310	0.1532	363.22	0.2693	0.1061
323.08	0.2469	0.1612	363.21	0.2877	0.1116
323.03	0.2658	0.1715	363.20	0.3096	0.1189
323.10	0.4550	0.2583	363.23	0.5731	0.1959
323.10	0.8445	0.4026	363.23	1.0235	0.3051
323.07	1.0836	0.4759	363.12	1.3810	0.3836
323.06	1.5792	0.5968	363.11	1.9372	0.4856

$$\ln(H_{2,1}/\text{MPa}) = (1.704 \pm 0.014) - (1568 \pm 39)[1/(T/\text{K}) - 1/333.15]$$

Solvent Chem. Abstracts name: 2,2-bis-[(1-oxonyl)oxylmethyl]-1,3-propanediyl ester of nonanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in Wahlström and Vamling.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the equation below the table.

Source and Purity of Material:
(1) Difluoromethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetrananoate. Synthesized from pentaerythriiol and nonanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%.

Estimated Error:
Uncertanties in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) Difluoromethane or HFC32; CH_2F_2; [75-10-5]
(2) Pentaerythritol tetra-2-ethylbutanoate; $C_{29}H_{52}O_8$; [139116-32-8]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 323.10–363.28
p_1 /MPa = 0.1180–1.7605

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mole Fraction x_1	T/K	p_1 /MPa	Mole Fraction x_1
			343.28	0.1382	0.0683
	The		343.26	0.1753	0.0859
	solvent		343.24	0.1894	0.0923
303.15	is a solid		343.27	0.4261	0.1915
	at this		343.27	0.8317	0.3311
	temperature		343.28	1.1018	0.4039
			343.28	1.5808	0.5127
323.11	0.1180	0.0817	363.25	0.1552	0.0677
323.11	0.1495	0.1024	363.23	0.1971	0.0726
323.10	0.1621	0.1112	363.28	0.2115	0.0776
323.11	0.3624	0.2243	363.22	0.4792	0.1646
323.11	0.7130	0.3897	363.22	0.9242	0.2893
323.11	0.9282	0.4548	363.15	1.2414	0.3607
323.11	1.3377	0.5716	363.25	1.7605	0.4613

$$\ln(H_{2,1}/\text{MPa}) = (1.696 \pm 0.008) - (1821 \pm 29)[1/(T/\text{K}) - 1/333.15]$$

Solvent Chem. Abstracts Name: 2,2-bis[(2-ethyl-1-oxobutoxy)methyl]-1,3-propanediyl ester of 2-ethyl butanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in Wahlström and Vamling.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) Difluoromethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylbutanoate. Synthesized from pentaerythriiol and 2-ethyl-butanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%. Melting point 310–312 K.

Estimated Error:
Uncertanites in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) Difluoromethane or HFC-32; CH_2F_2; [75-10-5]
(2) Pentafluoroethane or HFC-125; C_2HF_5; [354-33-6]

Original Measurements:
M. Y. Jung, C. N. Kim, Y. M. Park, and J. S. Yoo, J. Chem. Eng. Data **46**, 750–753 (2001).

Variables:
T/K = 268.15–308.15
p_t /kPa = 676.7–2189.4

Prepared By:
H. L. Clever

Experimental Values
Vapor-liquid equilibrium data for the HFC-32 + HFC-125 System

T/K	p_t /kPa	Mol fraction Liquid x_1	Mol fraction Vapor y_1	T/K	p_t /kPa	Mol fraction Liquid x_1	Mol fraction Vapor y_1
268.15	571.3	0.0000	0.0000	288.15	1248.0	0.6303	0.6601
	606.8	0.1966	0.2282	Cont	1267.9	0.7331	0.7536
	634.3	0.3494	0.3979		1281.0	1.0000	1.0000
	658.8	0.4929	0.5363				
	676.7	0.6265	0.6578	298.15	1380.6	0.0000	0.0000
	686.6	0.7323	0.7542		1453.0	0.1864	0.2213
	693.8	1.0000	1.0000		1533,8	0.3323	0.3794
					1596.6	0.4964	0.5325
278.15	785.4	0.0000	0.0000		1643.0	0.6273	0.6551
	833.1	0.1883	0.2185		1669.7	0.7312	0.7499
	872.2	0.3422	0.3827		1689.6	1.0000	1.0000
	905.2	0.4984	0.5361				
	929.4	0.6299	0.6603	308.15	1782.9	0.0000	0.0000
	943.8	0.7326	0.7548		1890.5	0.1763	0.2108
	951.8	1.0000	1.0000		1983.5	0.3391	0.3765
					2065.9	0.4953	0.5310
288.15	1052.8	0.0000	0.0000		2121.9	0.6237	0.6486
	1117.4	0.1928	0.2247		2158.9	0.7300	0.7469
	1170.2	0.3419	0.3845		2189.4	1.0000	1.0000
	1215.5	0.4975	0.5419				

Auxiliary Information

Method/Apparatus/Procedure:
A circulation method was used. The apparatus consists of an equilibrium unit, a sampling and analysis unit and a supply unit. The equilibrium unit consists of a stainless steel equilibrium cell of 128 cm^3 volume, a magnetic pump, and a constant temperature bath. Temperature was measured with a calibrated platinum resistance thermometer and the pressure with a quartz crystal pressure transducer. A ~0.1 cm^3 sample was analyzed by GC using a thermal conductivity detector.

Source and Purity of Material:
(1) Difluoromethane. Ulsan Chemical Co. Stated to be 99.8 mass %.
(2) Pentafluoroethane. DuPont Co. Stated to be 99.9 mass %.
Both components used as received.

Estimated Error:
δT/K = ±0.02
$\delta p_t/p_t$ = ±0.004
$\delta x_1/x_1 = \delta y_1/y_1$ = ±0.003

Components:
(1) Difluoromethane or R-32; CH_2F_2; [75-10-5]
(2) Polol ester mixture; $C(CH_2OOCR)_4$ with R of $n=5-10$; Mole wt 610.

Original Measurements:
Y. Takaishi and K. Oguchi, Proceedings-International Congress of Refrigeration, 19th, The Hague, August 1995, Vol. 4A, pp. 568–574.

Variables:
T/K=243.15–303.15
p_1 /MPa=0.270–1.905

Prepared By:
H. L. Clever

Experimental Values
Miscibility Limit for the R-32+polyol ester

Temperature (T/K)	Partial Pressure[a] (p_1 /MPa)	Weight Fraction w_1	Temperature (T/K)	Partial Pressure[a] (p_1 /MPa)	Weight Fraction w_1
243.15	0.270	0.308	283.15	1.085	0.420
243.15	0.273	0.940	283.15	1.101	0.903
			283.21	1.102	0.903[b]
253.15	0.395	0.323			
253.15	0.405	0.938	286.39	1.184	0.441[b]
254.79	0.419	0.324[b]	293.15	1.453	0.502
			293.15	1.461	0.872
263.15	0.570	0.343			
263.16	0.570	0.929	298.42	1.682	0.845[b]
273.15	0.794	0.375	299.77	1.739	0.603[b]
273.15	0.809	0.925			
			303.06	1.890	0.700[b]
			303.15	1.905	0.713
			303.15	1.905	0.713

[a]It is assumed the vapor phase contains R-32 only.
[b]Miscibility limit by visual inspection. Upper consolute point is at 303.2 K, 1.91 MPa and about 0.720 weight fraction R-32.

Measurements over the miscible range were shown in Fig. 2. The authors give correlation equations between R-32 pressure and R-32 weight fraction for each isotherm over the miscible range. The equations are:
For 243.15 K, $w_1=0-w_1=0.308$; $(p_1/\text{MPa})=1.5552w_1-2.303w_1^2$.
For 253.15 K, $w_1=0-w_1=0.328$; $(p_1/\text{MPa})=2.2719w_1-3.2477w_1^2$.
For 263.15 K, $w_1=0-w_1=0.343$; $(p_1/\text{MPa})=4.0963w_1-10.993w_1^2-11.354w_1^3$.
For 273.15 K, $w_1=0-w_1=0.375$; $(p_1/\text{MPa})=4.9532w_1-10.560w_1^2+7.9934w_1^3$.
For 283.15 K, $w_1=0-w_1=0.420$; $(p_1/\text{MPa})=6.3673w_1-12.626w_1^2+8.609w_1^3$.
For 293.15 K, $w_1=0-w_1=0.502$; $(p_1/\text{MPa})=7.3299w_1-8.5479w_1^2-9.3694w_1^3+17.524w_1^4$.
For 303.15 K, $w_1=0-w_1=0.713$; $(p_1/\text{MPa})=10.313w_1-19.856w_1^2+15.226w_1^3-3.3780w_1^4$.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental apparatus consists of a glass equilibrium cell of volume 17.93 cm^3, a temperature measuring system and a pressure measuring system. The apparatus is used to measure vapor pressure of pure liquids, solubility of refrigerant+oil mixtures and liquid-liquid phase separations if they occur. The apparatus is described in detail in an earlier paper.[1] The solubility and miscibility limit for R-32+polyol ester were measured over the complete composition range along seven isotherm between 243.15 K and 303.15 K and at pressures up to 2 MPa. All of the data are shown in Fig. 2 of the paper. The table above gives the values that define the immiscible region. It includes six miscibility limits observed visually. The weight fraction solubility of R-32 and the pressure in the miscible region are correlated along the seven isotherms by equations given above.

Source and Purity of Material:
(1) Difluoromethane or R-32. Source not given. Purity stated to be 99.99 wt %.
(2) Polyol ester lubricating oil. Kyodo Oil Technical Research Center Co., Ltd. Saitama, Japan. Mol. wt. 610; Density at 298.15 K is 974 kg m^{-3}; Kinematic viscosity: 313.15 K is 31 mm^2 s^{-1}, 373.15 K is 5
mm2 s−1.

Estimated Error:
δT/K=±0.010
δp_1 /kPa=±2
$\delta w_1/w_1=\pm 0.005$

References:
[1]Y. Takaishi, H. Nakagawa, and K. Oguchi, Trans. JAR **10**(1), 67–73 (1993).

3.8. Fluoromethane

Components:
(1) Fluoromethane; CH_3F; [593-53-3]
(2) Water; H_2O; [7732-16-5]

Evaluators:
Rubin Battino, Wright State University, Dayton, OH 45435
H. Lawrence Clever, Emory University, Atlanta, GA 30322
2002

Evaluation

An evaluation of the solubility of fluoromethane in water at a partial pressure of 0.101325 MPa from 273.15 K to 353.15 K.
Three papers report the solubility of fluoromethane in water. Glew and Moelwyn-Hughes[1] report nine values between 273.21 K and 353.40 K. Henry's law was tested at 303.15 K and maybe other temperatures as well. This is a complete and careful study. Swain and Thornton[3] report eight values, four near 302.6 K and four near 313.5 K. Rosenthal and Nickels[3] report one value at 310.15 K using a radioactive isotope method.
The 18 experimental values of the mole fraction solubility of fluoromethane in water were fit by a nonlinear regression to the three constant Clark, Glew, and Weiss (CGW) equation and to the three constant Benson and Krause equation (BK). After elimination of the 283.15 K value from Glew and Moelwyn-Hughes[1] and the 315.15 K value of Rosenthal and Nickels[3] very satisfactory fits were obtained to the 16 remaining values with both equations. Both equations are given here, but the CGW equation was chosen to calculate the recommended smoothed value of mole fraction solubility at 0.101325 MPa partial pressure, the Ostwald coefficients and the thermodynamic changes on solution in table.
The CGW equation is:
$\ln x_1=-(50.4960\pm1.7111)+(73.5668\pm2.4905)/(T/100\text{ K})+(17.3725\pm0.9017)\ln(T/100\text{ K})$, where x_1 is the mole fraction solubility of CH_3F at a partial pressure of 0.101325 MPa and (T/100 K) is the Kelvin temperature divided by 100 K. Ostwald coefficients and thermodynamic changes on solution were also calculated and they are given in Table 11 at five degree intervals from 273.15 K to 353.15 K. The fit $r^2=0.9995$ with a standard error of the fit of 0.0085.
The BK equation is:
$\ln x_1=-(4.7796\pm0.4366)-(3393.3505\pm269.6518)(T/\text{K})^{-1}+(828\,076.0404\pm41.614)(T/\text{K})^{-2}$, where x_1 is the mole fraction solubility of CH_3F in water at a
partial pressure of 0.101325 MPa and T is the Kelvin temperature. The fit $r^2=0.9994$ with a standard error of the fit of 0.0092.
The values are given in Table 11 and Fig. 3.

References
[1]D. N. Glew and E. A. Moelwyn-Hughes, Disc. Faraday Soc. **15**, 150–161 (1953).
[2]C. G. Swain and E. R. Thornton, J. Am. Chem. Soc. **84**, 822–826 (1962).
[3]M. S. Rosenthal and R. J. Nickels, Phys. Med. Biol. **30**, 945–950 (1985).

TABLE 11. The recommended mole fraction solubility of fluoromethane in water at a partial pressure of 0.101325 MPa and at five degree intervals from 273.15 K to 353.15 K. Also given are values of the Ostwald coefficient and the thermodynamic changes on solution

Temperature (T/K)	Mole fraction 10^3x_1	Ostwald Coefficient (L/cm^3 cm^{-3})	Enthalpy changes ($\Delta_{sln}H^o$/kJ mol^{-1})	Entropy changes ($\Delta_{sln}S^o$/J K^{-1} mol^{-1})	Heat capacity change ($\Delta_{sln}C^o_p$/J K^{-1} mol^{-1})
273.15	2.228	2.78_0	−21.71	−130.3	144
278.15	1.882	2.39_0	−20.94	−127.6	144
283.15	1.608	2.06_5	−20.27	−125.1	144
288.15	1.388	1.82_0	−19.54	−122.5	144
293.15	1.211	1.61_5	−18.82	−120.0	144
298.15	1.067	1.44_5	−18.10	−117,6	144
303.15	0.948	1.30_5	−17.38	−115.2	144
308.15	0.849	1.18_5	−16.66	−112.8	144
313.15	0.767	1.08_5	−15.94	−110.5	144
318.15	0.699	1.00_5	−15.21	−108.2	144
323.15	0.640	0.93_0	−14.49	−106.0	144
328.15	0.591	0.87_0	−13.77	−103.8	144
333.15	0.549	0.82_0	−13.05	−101.6	144
338.15	0.513	0.77_5	−12.33	−99.4	144
343.15	0.482	0.73_5	−11.60	−97.3	144
348.15	0.456	0.70_5	−10.88	−95.2	144
353.15	0.433	0.67_5	−10.16	−93.2	144

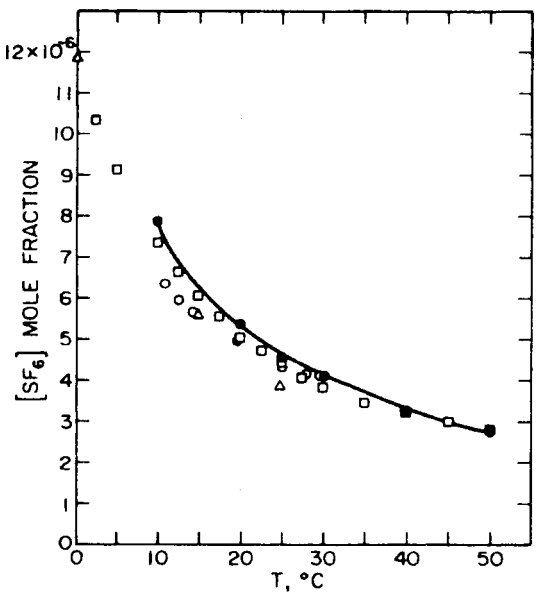

FIG. 3. The solubility of fluoromethane in water: $\ln x_1$ vs T/K. The fitted line and experimental points.

Components:
(1) Fluoromethane; CH_3F; [593-53-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. N. Glew and E. A. Moelwyn-Hughes, Disc. Faraday Soc. **15**, 150–161 (1953).

Variables:
T/K = 273.21–353.40
p_1 /kPa = 49.64–105.43 (at 303.18 K)

Prepared By:
H. L. Clever

Experimental Values

Solubility of CH_3F in water between 273.21 K and 353.40 K

T/K	Fluoromethane (p_1 /mmHg)	Fluoromethane (10^3c_1 /mol L^{-1})	Henry's Constant ($10^{-3}K$/mmHg L mol^{-1})	Mole Fraction 10^3x_1
273.21			6.13	2.229
283.34			8.83	1.551
293.34			11.41	1.201
298.21			12.92	1.062
303.18	372.3	25.43	14.64	
	389.5	26.61	14.64	
	406.7	27.75	14.66	
	425.9	29.00	14.69	
	445.0	30.27	14.70	
	539.6	36.79	14.67	
	553.3	37.81	14.63	
	569.2	38.87	14.64	
	603.2	41.18	14.65	
	640.6	43.66	14.67	
	681.0	46.88	14.65	
	702.0	47.95	14.64	
	723.2	49.42	14.63	
	745.2	51.00	14.61	
	766.8	52.50	14.64	
	790.8	54.00	14.64	
	—	—	Av. 14.65	0.938
313.05			17.94	0.772
322.64			21.6	0.641
333.23			25.4	0.548
353.40			32.5	0.433

The complete data set was given at only the one temperature of 303.18 K.

The authors fitted the Henry's constants to the equation:

$\log K = \log(p_1/\text{mmHg})/(c_1/\text{mol L}^{-1}) = 59.096 - 17.781 \log(T/\text{K}) - 3265.7/(T/\text{K})$.

The thermodynamic changes for the escape of one mole of CH_3F from the solution are: $\Delta H°$/kcal mol^{-1} = 4.404,

$\Delta S°$/cal K^{-1} mol^{-1} = 33.64,

ΔC°_p /cal K^{-1} mol^{-1} = −35.22.

The compiler calculated the mole fraction values assuming 1 L of solution had the same density as pure water.

The authors give the equation for the vapor pressure of fluoromethane.

$\log(p^\circ_1/\text{mmHg} = 21.794 - 5.238 \log(T/\text{K}) - 1328/(T/\text{K})$.

Term by term subtraction of the log (K/mmHg L mol^{-1}) equation from the previous page gives an equation from which one can calculate the CH_3F solubility, c°_1, at the gas saturation temperature.

Auxiliary Information

Method/Apparatus/Procedure:

A gas buret and absorption pipet were kept at constant temperature by circulation of thermostated water. They were connected by flexible copper tubing, with machined metal joints. The glass taps were grease free and mercury sealed. The amount of gas absorbed by a known weight of water was determined by measuring the volume of gas absorbed at a definite temperature and pressure. The partial pressures of the halide are given in mmHg at 25 °C and the concentration of the halide are given in moles of solute per liter of solution at the temperature T.

Source and Purity of Material:

(1) Fluoromethane. Prepared by damp distillation of potassium fluoride and potassium methyl sulfate at 200 °C–220 °C. Purified by passage through 33% aq KOH and conc. H_2SO_4. Recycled until vapor pressure reached 754 −8 mmHg at −78.51 °C. The analysis indicated a purity better than 99.8%.[1]
(2) Water. Distilled. Deionized and vigorously boiled at room temperature to degas.

Estimated Error:
$\delta K/K = \pm 0.005$ (compiler).

References:
[1]D. N. Glew and E. A. Moelwyn-Hughes, Proc. R. Soc. London, Ser. A **211**, 254 (1952).

Components:
(1) Fluoromethane; CH_3F; [593-53-3]
(2) Water; H_2O; [7732-18-5]
(2) Water-d_2; D_2O; [7789-20-0]

Original Measurements:
C. G. Swain and E. R. Thornton, J. Am. Chem. Soc. **84**, 822–826 (1962).

Variables:
T/K = 302.60 and 313.50

Prepared By:
H. L. Clever

Experimental Values

Solubility of CH_3F in water and heavy water at 302.60 K and 313.50 K

t/°C	T/K	Henry's Constant (10^4k/mmHg L mol^{-1})	Henry's Constant (H/MPa)	Mole Fraction 10^4x_1
		H_2O		
29.44	302.59	1.440	105.7	9.59
29.42	302.57	1.410	103.5	9.79
29.45	302.60	1.431	105.1	9.64
29.45	302.60	1.431	105.1	9.64
40.34	313.49	1.804	132.5	7.65
40.35	313.50	1.794	131.7	7.69
40.35	313.50	1.832	134.5	7.53
40.35	313.50	1.829	134.3	7.55
		D_2O		
29.42	302.57	1.396	102.5	9.89
29.45	302.60	1.401	102.9	9.85
29.45	302.60	1.416	104.0	9.74
40.34	313.49	1.743	127.5	7.95
40.34	313.49	1.714	125.4	8.08
40.35	313.50	1.747	127.8	7.93

The compiler calculated the Henry's constant, H/MPa = (p_1 /MPa)/x_1 and the mole fraction solubility at 0.101325 MPa.

Auxiliary Information

Method/Apparatus/Procedure:

The authors give a detailed description in the paper. The solvents were degassed by heating to 70–100 °C and pumping on for 5–10 min periods as the solvent cooled. This was repeated over a number of days. The solvent was vacuum distilled into the equilibrium cell. The solvent was weighed to the nearest 0.01 g. The gas volume was known and its pressure measured. Both gas and solvent were cooled to liquid N_2 temperatures and then contacted and brought to the measurement temperature and equilibrium established. The total gas moles and the gas moles in the vapor could be calculated from the ideal gas law.

Source and Purity of Material:

(1) Fluoromethane. Prepared by authors by reaction of iodomethane with silver fluoride. Washed with aqueous KOH and concentrated H_2SO_4. Stored in stainless steel cylinder.
(2) Water. Distilled water distilled again from $KMnO_4$.
(2) Water-d_2. Liquid Carbonic Co. Purity >99.5%.

Estimated Error:
δT/K = ±0.01
δp_1 /mmHg = ±0.05

Components:
(1) Fluoro-18-methane; $CH_3{}^{18}F$; [3832-44-8]
(2) Water; H_2O; [7732-18-5]
(2) Paraffin oil
(2) Bone

Original Measurements:
M. S. Rosenthal and R. J. Nickels, Phys. Med. Biol. **30**, 945–950 (1985).

Variables:
T/K = 310

Prepared By:
H. L. Clever

Experimental Values

Solubility of $CH_3{}^{18}F$ in water, paraffin oil and bone at 310 K

Temperature		Solvent	Ostwald Coefficient
(t/°C)	(T/K)		(L/cm^3 cm^{-3})
37	310	Water	1.19 ± 0.07
		Paraffin oil	1.24 ± 0.07
		Bone	0.25 ± 0.11

The results are the average of 10–20 measurements.

The authors estimated the bone-blood partition coefficient to be 0.21 ± 0.08 from the bone Ostwald coefficient above and a blood fluoromethane solubility from the literature.

A gas chromatographic technique using a semi-wet bone column gave an Ostwald solubility of 0.14 ± 0.01 for bone + CH_3F which the authors consider in satisfactory agreement with the value above.

Auxiliary Information

Method/Apparatus/Procedure:
The solubilities were measured using the fluoro-18-methane, a positron emitter. About 7 mL of solvent was placed in a 14 mL tube with a septa cap. About 370 kBq (10 μCi) of gas was introduced. The tubes were vigorously shaken for 2 min then rotated at 37 °C for 10 min–2 h. The tube was placed between two shielded BaF_2 crystals and both liquid and vapor phase were counted an equal time for single and coincident events which were corrected for decay.
The bone, cow femur, was cleaned of tissue, fat, and marrow. Degreased in chromic acid and the wet bone ground to 600–425 μm (30–40 mesh). The bone was suspended in water. The final result was corrected for the gas solubility in water.

Source and Purity of Material:
(1) Fluoro-18-methane. Prepared at the University of Wisconsin using the tandem van de Graaf accelerator.
(2) Water. Deionized and distilled.
Paraffin oil. Nothing specified.
Bone. See comments under method.

Estimated Error:
δT/K = ± 1
Ostwald coefficients, see standard deviations in table.

Components:
(1) Fluoromethane; CH_3F; [593-53-3]
(2) Methanol; CH_3OH; [67-56-1]

Original Measurements:
C. S. O. Silva, I. M. A. Fonseca, and L. Q. Lobo, Fluid Phase Eq. **135**, 137–144 (1996).

Variables:
T/K = 288.82–300.21
p_1 /MPa = 0.101325

Prepared By:
H. L. Clever

Experimental Values

Solubility of fluoromethane in methanol from 288.82 to 300.21 K at a partial pressure of 0.101325 MPa (1 atm)

T/K	Mole fraction $10^3 x_1$	Ostwald Coefficient (L/cm^3 cm^{-3})	Henry's Constant ($H_{1,2}$ /MPa)
288.82	1.535	0.979	66.00
291.15	1.228	0.796	82.53
293.48	0.843	0.557	120.2
295.29	0.559	0.375	181.1
298.66	0.312	0.216	324.9
300.21	0.116	0.082	872.1

The authors fitted their mole fraction values to the equation: $R \ln x_1 = 146\,187.8 - 6302.640/(T/\mathrm{K}) - 21\,959.75 \ln(T/\mathrm{K})$.

The thermodynamic changes for the solution process are: ΔH/kJ mol^{-1} = −244.7 and ΔS/J K^{-1} mol^{-1} = −889.75 both at 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental method was a modification of the method of Kaszonyi *et al.*[1] The solvent was degassed by a combination of the techniques described by Gibbs and Ness[2] and by Bell *et al.*[3]
The whole apparatus is evacuated, the gas is introduced, and the pressure is adjusted to atmospheric pressure. The alcohol sample is introduced into the absorption vessel and the vessel is shaken for 10–15 min. The mercury levels are equal in the three branches. The change in the mercury level is measured at least 8 h later to insure that equilibrium has been reached. The apparatus and method were checked by measuring the solubility of carbon dioxide and of nitrous oxide in water. Results agreed with literature values within 3%.

Source and Purity of Material:
(1) Fluoromethane. Matheson Co. Stated to be 99.5 mole % pure.
(2) Methanol. Riedel-de Haen. Minimum purity stated to be 99.63 mol %.

Estimated Error:
δT/K = ± 0.01
δp/mmHg = ± 0.01
$\delta x_1 / x_1$ = ± 0.03

References:
[1]A. Kaszonyi, M. Harustiak, and J. Kizlimk, J. Chem. Eng. Data **37**, 37 (1992).
[2]R. E. Gibbs and H. C. Van Ness, Ind. Eng. Fundam. **11**, 410 (1972).
[3]T. N. Bell, E. L. Cussler, K. R. Harris. C. N. Pepela, and P. J. Dunlap, J. Phys. Chem. **72**, 4693 (1968).

Components:
(1) Fluoromethane; CH_3F; [593-53-3]
(2) Ethanol; CH_3CH_2OH; [64-17-5]

Original Measurements:
C. S. O. Silva, I. M. A. Fonseca, and L. Q. Lobo, Fluid Phase Eq. **135**, 137–144 (1996).

Variables:
T/K = 283.90–301.51
p_1 /MPa = 0.101325

Prepared By:
H. L. Clever

Experimental Values

Solubility of fluoromethane in ethanol from 283.90 K to 301.51 K at a partial pressure of 0.101325 MPa (1 atm)

T/K	Mole Fraction 10^3x_1	Ostwald Coefficient (L/cm^3 cm^{-3})	Henry's Constant ($H_{1,2}$ /MPa)
283.90	2.076	0.870	48.80
285.71	1.981	0.837	51.14
288.30	1.999	0.856	50.70
290.37	1.948	0.843	52.02
292.70	2.243	0.984	45.18
293.74	2.249	0.993	45.05
294.52	2.133	0.946	47.51
297.11	1.841	0.830	55.05
298.92	1.453	0.663	69.74
301.51	1.124	0.523	90.14

The authors fitted their mole fraction values to the equation: $R \ln x_1 = 45\,413.1 - 1975.268/(T/\mathrm{K}) - 6817.18 \ln(T/\mathrm{K})$.

The thermodynamic changes for the solution process are: ΔH/kJ mol^{-1} = −57.274 and ΔS/J K^{-1} mol^{-1} = −245.62 both at 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental method was a modification of the method of Kaszonyi *et al.*[1] The solvent was degassed by a combination of the techniques described by Gibbs and Ness[2] and by Bell *et al.*[3]
The whole apparatus is evacuated, the gas is introduced, and the pressure is adjusted to atmospheric pressure. The alcohol sample is introduced into the absorption vessel and the vessel is shaken for 10–15 min. The mercury levels are equal in the three branches. The change in the mercury level is measured at least 8 h later to insure that equilibrium has been reached. The apparatus and method were checked by measuring the solubility of carbon dioxide and of nitrous oxide in water. Results agreed with literature values within 3%.

Source and Purity of Material:
(1) Fluoromethane. Matheson Co. Stated to be 99.5 mole % pure.
(2) Ethanol. Riedel-de Haen. Minimum purity stated to be 99.6 mol %.

Estimated Error:
δT/K = ±0.01
δp/mmHg = ±0.01
$\delta x_1 / x_1$ = ±0.03

References:
[1]A. Kaszonyi, M. Harustiak, and J. Kizlimk, J. Chem. Eng. Data **37**, 37 (1992).
[2]E. Gibbs and H. C. Van Ness, Ind. Eng. Fundam. **11**, 410 (1972).
[3]T. N. Bell, E. L. Cussler, K. R. Harris. C. N. Pepela, and P. J. Dunlap, J. Phys. Chem. **72**, 4693 (1968).

Components:
(1) Fluoromethane; CH_3F; [593-53-3]
(2) 1-Propanol; $CH_3CH_2CH_2OH$; [71-23-8]

Original Measurements:
C. S. O. Silva, I. M. A. Fonsecs, and L. Q. Lobo, Fluid Phase Eq. **135**, 137–144 (1996).

Variables:
T/K = 284.94–300.21
p_1 /MPa = 0.101325

Prepared By:
H. L. Clever

Experimental Values

Solubility of fluoromethane in 1-propanol from 284.94 K to 300.21 K at a partial pressure of 0.101325 MPa (1 atm)

T/K	Mole Fraction 10^3x_1	Ostwald Coefficient (L/cm^3 cm^{-3})	Henry's Constant ($H_{1,2}$ /MPa)
284.94	3.038	0.975	33.35
286.49	2.742	0.884	36.95
288.55	2.819	0.915	35.94
291.41	2.778	0.911	36.47
292.45	2.927	0.964	34.61
293.48	2.883	0.953	35.15
296.07	2.893	0.965	35.02
298.66	2.663	0.898	38.05
300.21	2.622	0.890	38.64

The authors fitted their mole fraction values to the equation: $R \ln x_1 = 5030.9 - 219.230/(T/\mathrm{K}) - 762.55 \ln(T/\mathrm{K})$.

The thermodynamic changes for the solution process are: ΔH/kJ mol^{-1} = −8.124 and ΔS/J K^{-1} mol^{-1} = −76.35 both at 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental method was a modification of the method of Kaszonyi *et al.*[1] The solvent was degassed by a combination of the techniques described by Gibbs and Ness[2] and by Bell *et al.*[3]
The whole apparatus is evacuated, the gas is introduced, and the pressure is adjusted to atmospheric pressure. The alcohol sample is introduced into the absorption vessel and the vessel is shaken for 10–15 min. The mercury levels are equal in the three branches. The change in the mercury level is measured at least 8 h later to insure that equilibrium has been reached. The apparatus and method were checked by measuring the solubility of carbon dioxide and of nitrous oxide in water. Results agreed with literature values within 3%.

Source and Purity of Material:
(1) Fluoromethane. Matheson Co. Stated to be 99.5 mole % pure.
(2) 1-Propanol. Riedel-de Haen. Minimum purity stated to be 99.97 mol %.

Estimated Error:
δT/K = ±0.01
δp/mmHg = ±0.01
$\delta x_1 / x_1$ = ±0.03

References:
[1]A. Kaszonyi, M. Harustiak, and J. Kizlimk, J. Chem. Eng. Data **37**, 37 (1992).
[2]R. E. Gibbs and H. C. Van Ness, Ind. Eng. Fundam. **11**, 410 (1972).
[3]T. N. Bell, E. L. Cussler, K. R. Harris. C. N. Pepela, and P. J. Dunlap, J. Phys. Chem. **72**, 4693 (1968).

Components:
(1) Fluoromethane; CH_3F; [593-53-3]
(2) 1-Butanol; $CH_3CH_2CH_2CH_2OH$; [71-36-3]

Original Measurements:
C. S. O. Silva, I. M. A. Fonsecs, and L. Q. Lobo, Fluid Phase Eq. **135**, 137–144 (1996).

Variables:
T/K=281.07–300.47
p_1 /MPa=0.101325

Prepared By:
H. L. Clever

Experimental Values

Solubility of fluoromethane in 1-butanol from 281.07 K to 300.47 K at a partial pressure of 0.101325 MPa (1 atm).

T/K	Mole fraction 10^3x_1	Ostwald coefficient (L/cm^3 cm^{-3})	Henry's constant ($H_{1,2}$ /MPa)
281.07	3.136	0.807	32.31
283.38	3.567	0.925	28.40
286.23	3.176	0.831	31.91
288.56	3.309	0.872	30.62
291.41	3.386	0.901	29.92
292.70	3.724	0.945	27.21
293.22	3.537	0.947	28.65
295.81	3.115	0.841	32.53
298.66	2.932	0.799	34.56
300.47	2.903	0.797	34.91

The authors fitted their mole fraction values to the equation: $R \ln x_1 = 13\,619.5 - 592.100/(T/\mathrm{K}) - 2050.283 \ln(T/\mathrm{K})$.

The thermodynamic changes for the solution process are: ΔH/kJ mol^{-1} = −19.192 and ΔS/J K^{-1} mol^{-1} = −112.49 both at 298.15 K.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental method was a modification of the method of Kaszonyi *et al.*[1] The solvent was degassed by a combination of the techniques described by Gibbs and Ness[2] and by Bell *et al.*[3]
The whole apparatus is evacuated, the gas is introduced, and the pressure is adjusted to atmospheric pressure. The alcohol sample is introduced into the absorption vessel and the vessel is shaken for 10–15 min. The mercury levels are equal in the three branches. The change in the mercury level is measured at least 8 h later to insure that equilibrium has been reached. The apparatus and method were checked by measuring the solubility of carbon dioxide and of nitrous oxide in water. Results agreed with literature values within 3%.

Source and Purity of Material:
(1) Fluoromethane. Matheson Co. Stated to be 99.5 mol % pure.
(2) 1-Butanol. Riedel-de Haen. Minimum purity stated to be 99.97 mol %.

Estimated Error:
δT/K = ±0.01
δp/mmHg = ±0.01
$\delta x_1/x_1$ = ±0.03

References:
[1]A. Kaszonyi, M. Harustiak, and J. Kizlimk, J. Chem. Eng. Data **37**, 37 (1992).
[2]R. E. Gibbs and H. C. Van Ness, Ind. Eng. Fundam. **11**, 410 (1972).
[3]T. N. Bell, E. L. Cussler, K. R. Harris. C. N. Pepela, and P. J. Dunlap, J. Phys. Chem. **72**, 4693 (1968).

3.9. Hexafluoroethane

Components:
(1) Hexafluoroethane; C_2F_6; [76-16-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–246 (1979).

Variables:
T/K=278.15–303.15
p_{tot} /MPa=0.1013

Prepared By:
H. L. Clever

Experimental Values

Solubility of hexafluoromethane in water from 278.15 K to 303.15 K at 0.1013 MPa

t/°C	T/K	Mole fraction 10^6x_1	Std. Dev. $10^6\sigma$	Ostwald coefficient (10^3L/mL mL^{-1})	Std. Dev. $0.10^3\sigma$	No. of det'n
5	278.15	2.15	0.03	2.69	0.03	3
10	283.15	1.73	0.01	2.22	0.02	3
15	288.15	1.45	0.01	1.88	0.02	3
20	293.15	1.15	0.01	1.51	0.01	3
25	298.15	1.03	0.01	1.38	0.01	4
30	303.15	0.942	0.019	1.29	0.03	4

The authors fitted their data to equations in mole fraction and the Ostwald coefficient.

$$R \ln[x_1/(p_1/\mathrm{MPa})] = -318.510 + 17\,768.0/(T/\mathrm{K}) + 40.6345 \ln(T/\mathrm{K}) \quad (\sigma = 0.63\%)$$

$$R \ln(L/\mathrm{mL\ mL^{-1}}) = -300.081 + 17\,103.8/(T/\mathrm{K}) + 40.3030 \ln(T/\mathrm{K}) \quad (\sigma = 1.01\%).$$

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and procedure were similar to that described by Ben-Naim and Baer[1] as modified by Wen and Hung.[2] It consists of a mercury manometer, a gas-volume measuring buret, a dissolution cell of 2.1 or 2.4 L, and a mercury reservoir. The apparatus is immersed in a water thermostat. Degassing is done with a Battino *et al.*[3] type apparatus. The cell containing the solvent is degassed, the system filled with solvent saturated gas to 1 atm total pressure. The solvent is stirred, as the gas dissolves the pressure is maintained at 1 atm until equilibrium is reached.

Source and Purity of Material:
(1) Hexafluoroethane. Matheson Gas Products. Minimum purity of 99.6% was confirmed by GLC. Used as received.
(2) Water. Distilled then passed through Milli-Q system.

Estimated Error:
δT/K = ±0.005
δp/Torr = ±3
$\delta L/L$ = ±0.0064 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]W.-Y. Wen and J. H. Hung, J. Phys. Chem. **74**, 170 (1970).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 896 (1971).

Components:
(1) Hexafluoroethane or Freon-116; C_2F_6; [76-16-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. Park, T. R. Rettich, R. Battino, D. Peterson, and E. Wilhelm, J. Chem. Eng. Data **27**, 324–326 (1982).

Variables:
T/K = 298.15
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_6 in water at 298.15 K and 101.325 kPa

T/K	No. of Determinations	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Standard Deviation
298.15	5	0.001206	6.4

The Bunsen coefficient was measured on the modified apparatus 1.

The standard deviation is given as per cent standard deviation, $100\sigma/\alpha$.

Auxiliary Information

Method/Apparatus/Procedure:
Two different versions of the Scholander[1] microgasometric apparatus were used. They were housed in an air thermostat. Apparatus 1 was the modified form described by Douglas[2] and by others.
The authors modified Apparatus 2. The design includes a more efficient method of degassing and transferring water to the apparatus. The apparatus itself had a 4 cm^3 compensation chamber, a 10 cm^3 equilibration chamber, and an 8 cm side arm.

Source and Purity of Material:
(1) Freon-116. Air Products Co. Stated to be 99.6 mol % minimum purity.
(2) Water. House distilled (reverse osmosis), passed through an ion exchange column until specific resistance was 5×10^6 Ω cm.

Estimated Error:
δT/K = ±0.05
Solubility. See percent standard deviation above.

References:
[1]P. F. Scholander, J. Biol. Chem. **167**, 235 (1947).
[2]E. Douglas, J. Phys. Chem. **68**, 169 (1964).

Components:
(1) Hexafluoroethane; C_2F_6; [76-16-4]
(2) Water-d_2; D_2O; [7789-20-0]

Original Measurements:
W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–246 (1979).

Variables:
T/K = 278.15–298.15
p_{tot} /MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Solubility of hexafluoroethane in water-d_2 from 278.15 K to 298.15 K at 0.1013 MPa

t/°C	T/K	Mole Fraction $10^6 x_1$	Std. Dev. ($10^6\sigma$)	Ostwald Coefficient ($10^3 L$/mL mL^{-1})	Std. Dev. $10^3\sigma$	No. of det'n
5	278.15	2.83	0.01	3.62	0.01	3
10	283.15	2.26	0.02	2.87	0.03	3
15	288.15	1.69	0.03	2.19	0.04	2
20	293.15	4.79	–	1.82	–	1
25	298.15	1.17	–	1.57	–	1

The authors fitted their data to equations in mole fraction and the Ostwald coefficient.

$$R \ln[x_1/(p_1/\text{MPa})] = -1300.70 + 61\,228.0/(T/\text{K}) + 187.482 \ln(T/\text{K}) \quad (\sigma = 0.78\%)$$

$$R \ln(L/\text{mL mL}^{-1}) = -1277.17 + 60\,330.4/(T/\text{K}) + 186.393 \ln(T/\text{K}) \quad (\sigma = 1.14\%).$$

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and procedure were similar to that described by Ben-Naim and Baer[1] as modified by Wen and Hung.[2] It consists of a mercury manometer, a gas-volume measuring buret, a dissolution cell of 2.1 or 2.4 L, and a mercury reservoir. The apparatus is immersed in a water thermostat. Degassing is done with a Battino *et al.*[3] type apparatus. The cell containing the solvent is degassed, the system filled with solvent saturated gas to 1 atm total pressure. The solvent is stirred, as the gas dissolves the pressure is maintained at 1 atm until equilibrium is reached.

Source and Purity of Materials:
(1) Hexafluoroethane. Matheson Gas Products. Minimum purity of 99.6% was confirmed by GLC. Used as received.
(2) Water-d_2. Stohler Isotope Chemicals Co. Specified to be 99.8%. Used as received.

Estimated Error:
δT/K = ±0.005
δp/Torr = ±3
$\delta L/L$ = ±0.0064 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]W.-Y. Wen and J. H. Hung, J. Phys. Chem. **74**, 170 (1970).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 896 (1971).

Components:
(1) Hexafluoroethane; C_2F_6; [76-16-4]
(2) Water; H_2O; [7732-18-5]
(2) Tris-HCl buffer
(2) Liquid biolayers (two).

Original Measurements:
R. A. Smith, E. G. Porter, and K. W. Miller, Biochim. Biophys. Acta **645**, 327–328 (1981).

Variables:
TK=283.6, 298.2
p_1 /MPa=2.81

Prepared By:
H. L. Clever

Experimental Values

Solvent	Temperature (t/°C)	Temperature (T/K)	Partial Pressure (P_1 /atm)	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]
Water; H_2O; [7732-18-5] (estimated)	10.4	283.6	27.7	0.0081
	25.0	298.2	27.7	0.0050
Buffer. 0.15 mol L^{-1}KCl; [7447-40-7]				
0.1 wt % Na(N_3); [26628-23-8]	10.4	283.6	27.7	0.0070
10 mmol L^{-1} Tris-HCl; [1185-53-1]	25.0	298.2	27.7	0.0043
pH=7.4				
Egg phosphatidylcholine, 96%	10.4	283.6	27.7	0.440
Phosphatidic acid, 4%.	25.0	298.2	27.7	0.342
Egg phosphatidylcholine, 64%	10.5	283.6	27.7	0.412
Phosphatidic acid, 3%/cholesterol, 33%	25.0	298.2	27.7	0.333

The water solubility was estimated from a plot of ΔE_{vap} vs the log (solubility) of several known fluorocarbon gases in water.

Auxiliary Information

Method/Apparatus/Procedure:
Author's apparatus II.[1] Six 18 mL glass cuvetts, each fitted with a Teflon coated magnetic stirring button equipped with a stainless steel wire that broke the surface, are mounted inside a 50 mm ID pressure cylinder. Six stainless steel tubes, 0.26 μL mm^{-1}, passed through the disc top of the pressure vessel with one tube going to the bottom of each cuvett. The cuvetts contained either water, buffer or one of the two phospholipid suspensions. The pressure chamber was flushed with the gas, sealed and pressurized with the gas. After 12 h for equilibration, the cuvetts were sampled in turn by slowly bleeding 0.75 mL of solution at 0.5 mL m^{-1} through a 300 μL sample loop with a micrometer metering valve. The sample loop was decompressed and its contents flushed into a stripping device. The stripped gas went to a gas chromatograph for analysis.

Source and Purity of Materials:
(1) Hexafluoroethane. Nothing specified.
(2) Water and buffer. Nothing specified.
(2) Egg phosphatidylcholine and egg phosphtidic acid. Lipid Products, Nutfield. Cholesterol. Sigma Chemical Co. Recrystallized from methanol. The phospholipids, with or without cholesterol, were dried down from $CHCl_3$ solution and suspended in the buffer by vortexing and then sonification. Centrifugation yielded translucent suspensions of 10–46 mg mL^{-1}.

Estimated Error:
δT/K=±0.1
$\delta\alpha/\alpha$=±0.035–0.05 (compiler).

References:
[1]K. W. Miller, L. Hammond, and E. G. Porter, Chem. Phys. Lipids **20**, 229 (1977).

Components:
(1) Hexafluoroethane; C_2F_6; [76-16-4]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:
K. W. Miller, J. Phys. Chem. **72**, 2248–2249 (1968).

Variables:
T/K=280.15–305.45
p_1 /kPa=101.325

Prepared By:
H. L. Clever

Experimental Values

Temperature (t/°C)	Temperature (T/K)	Mole fraction 10^3x_1	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
7.8	280.15	2.537	0.536	0.550
12.8	285.95	2.556	0.536	0.561
18.7	291.85	2.500	0.520	0.556
25.0	298.15	2.451	0.506	0.552
32.3	305.45	2.387	0.489	0.547

The compiler calculated the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior. The compiler also added the Kelvin temperatures.

Smoothed data for use between 280.15 K and 305.45 K: $\ln x_1 = 31.2060 - 51.3086/(T/100\ \mathrm{K}) - 18.3124 \ln(T/100\ \mathrm{K})$.

The standard error about the regression line is 1.76×10^{-5}.

T/K	Mole Fraction 10^3x_1
283.15	2.543
288.15	2.528
293.15	2.499
298.15	2.459
303.15	2.409

Auxiliary Information

Method/Apparatus/Procedure:
The liquid is saturated with the gas at 1 atm partial pressure. The apparatus is that described by Dymond and Hildebrand.[1] It uses an all-glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressure.

Source and Purity of Materials:
(1) Hexafluoroethane. Matheson Co. Dried before use.
(2) Cyclohexane. Matheson, Coleman and Bell Co. "Spectroquality." Used as received.

Estimated Error:
Nothing specified.

References:
[1]J. H. Dymond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Hexafluoroethane; C_2F_6; [76-16-4]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:
D. F. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753–760 (1971).

Variables:
T/K = 297.25, 297.26
p/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of hexafluorobenzene in benzene

T/K	Mol Fraction 10^3x_1	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
297.25	1.111	0.278	0.303
297.26	1.102	0.277	0.301

The authors adjusted the gas solubility values to a gas partial pressure of 101.325 kPa (1 atm) by Henry's law. The compiler calculated the Bunsen coefficients.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3] Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred and the vacuum applied intermittently through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm. Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas and solvent vapor at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volume in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Materials:
(1) Hexafluoroethane. Either Matheson Co. or Air Products and Chemicals Co. Purest grade available, minimum purity greater than 99.0 mole % (usually only >95.9 mole %).
(2) Benzene. Mallinckrodt Co. Thiophene-free, analytical reagent grade. Used as received.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1/x_1$ = ±0.005

References:
[1]T. J. Morission and F. Billett, J. Chem. Soc. 2033, (1948).
[2]R. Battino, F. D. Evans, and F. D. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Hexafluoroethane; C_2F_6; [76-16-4]
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane or Freon 113; $C_2Cl_3F_3$; [76-13-1]

Original Measurements:
R. G. Linford and J. H. Hildebrand, Trans. Faraday Soc. **66**, 577–581 (1970).

Variables:
T/K = 275.40–300.73
p_1/kPa = 101.325

Prepared By:
H. L. Clever and P. L. Long

Experimental Values

Solubility of hexafluoroethane in 1,1,2-trichloro-1,2,2-trifluoroethane at a partial pressure of 0.101325 MPa between 275.40 K and 300.73 K

Temperature (t/°C)	T/K	Mole Fraction 10^2x_1	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
2.25	275.40	2.014	3.97	4.00
8.61	281.76	1.884	3.68	3.80
14.10	287.25	1.719	3.32	3.49
20.12	293.27	1.597	3.06	3.29
25.00	298.15	1.493	2.83	3.09
27.58	300.73	1.452	2.76	3.04

The compiler calculated the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior. The compiler also added the Kelvin temperatures.

Smoothed data for use between 275.40 K and 300.73 K: $\ln x_1 = -7.8393 + 10.8570/(T/100\ \text{K})$.

The standard error about the regression line is 1.69×10^{-4}.

T/K	Mole Fraction 10^2x_1
278.15	1.953
288.15	1.704
298.15	1.503

Auxiliary Information

Method/Apparatus/Procedure:
The liquid is saturated with the gas at 1 atm partial pressure. The apparatus is that described by Dymond and Hildebrand.[1] It uses an all-glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressure.

Source and Purity of Materials:
(1) Hexafluoroethane. Source not given. Stated to be purest commercially available sample. Dried before use.
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane. Matheson, Coleman and Bell Co. "Spectroquality." Used as received.

Estimated Error:
$\delta x_1/x_1$ = ±0.005

References:
[1]J. H. Dymond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Hexafluoroethane; C_2F_6; [76-16-4]
(2) Benzene; C_6H_6; [71-43-2]
(3) 1,1,2-Trichloro-1,2,2-trifluoroethane or Freon 113; $C_2Cl_3F_3$; [76-13-1]

Original Measurements:
R. G. Linford and J. H. Hildebrand, J. Phys. Chem. **73**, 4410–4411 (1969).

Variables:
T/K = 275.40–300.73
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of hexafluorobenzene in benzene + 1,1,2-trichloro-1,2,2-trifluoroethane at 298.15 K and a partial pressure of 0.101325 MPa

Benzene Mole Fraction x_2	Mole Fraction $10^3 x_1$	Bunsen Coefficient [α/cm^3 (STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
0.000	14.94	2.84	3.10
0.359	8.58	–	–
0.674	4.055	–	–
1.000	1.106	0.278	0.303

The compiler calculated the Bunsen and Ostwald coefficients assuming ideal gas behavior and Henry's law is obeyed.

Auxiliary Information

Method/Apparatus/Procedure:
The liquid is saturated with the gas at 1 atm partial pressure. The apparatus is that described by Dymond and Hildebrand.[1] It uses an all-glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressure.

Source and Purity of Materials:
(1) Hexafluoroethane. Source not given. Stated to be purest commercially available sample. Dried before use.
(2) Benzene.
(3) 1,1,2-Trichloro-1,2,2-trifluoroethane. Both (2) and (3) from Matheson, Coleman and Bell Co. "Spectroquality." Used as received.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.005$

References:
[1]J. H. Dymond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Hexafluoroethane; C_2F_6; [76-16-4]
(2) Hexafluorobenzene; C_6F_6; [392-56-3]

Original Measurements:
D. F. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753–760 (1971).

Variables:
T/K = 297.60, 298.1226
p/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

T/K	Mol Fraction $10^3 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
297.60	15.27	3.00	3.27
298.12	15.59	3.00	3.34

The authors adjusted the gas solubility values to a gas partial pressure of 101.325 kPa (1 atm) by Henry's law. The compiler calculated the Bunsen coefficients.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino *et al.*[2] The degassing apparatus is that described by Battino *et al.*[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred and the vacuum applied intermittently through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm. Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas and solvent vapor at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volume in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Materials:
(1) Hexafluoroethane. Either Matheson Co. or Air Products and Chemicals Co. Purest grade available, minimum purity greater than 99.0 mole % (usually only >95.9 mole %).
(2) Hexafluorobenzene. Imperial Smelting Co., Avnomouth, UK. GC purity 99.7%, density, $\rho_{298.15}$ = 1.60596 g cm^{-3}. Purification described in Anal. Chem. **40**, 224 (1968).

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1 / x_1 = \pm 0.005$

References:
[1]T. J. Morission and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and F. D. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Hexafloroethane; C_2F_6; [76-16-4]
(2) 1,1,2,2,3,3,4,4,4-Nonafluoro-*N*,*N*-bis(nonafluorobutyl)-1-butanamine or perfluorotributylamine; $C_{12}F_{27}N$; [311-89-7]

Original Measurements:
R. J. Powell, J. Chem. Eng. Data **17**, 302–304 (1971).

Variables:
T/K = 288.15–318.15
p/kPa = 101.325

Prepared By:
P. L. Long and H. L. Clever

Experimental Values

T/K	Mol Fraction $10^4 x_1$	Bunsen Coefficient [α/cm^3(STP)cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})	Slope N ($R\Delta \log x_1/\Delta \log T$)
298.15	74.8	3.13	3.42	−9.70

The compiler calculated the Bunsen and Ostwald coefficients, assuming an ideal gas and Henry's law behavior.

The author states that the solubility measurements were made over the temperature interval of about 288.15–318.15 K. Only the solubility value of 298.15 K was given in the paper. The slope, $N = R(\Delta \log x_1/\Delta \log T)$ was given.

Smoothed data for use between 288.15 K and 318.15 K. The compiler calculated smoothed data from the author's slope and solubility value at 298.15 K. The slope equation was rearranged:

$$\log x_1 = \log(0.04748) - (9.70R)\log[(T/\mathrm{K})/298.15] \text{ with } R = 1.9872 \text{ cal K}^{-1}\text{ mol}^{-1}.$$

T/K	Mol Fraction x_1
288.15	0.05608
298.15	0.04748
308.15	0.04042
318.15	0.03458

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is the Diamond and Hildebrand[1] apparatus which uses an all glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final pressures. The solvent is degassed by freezing, pumping and followed by boiling under reduced pressure.

Source and Purity of Materials:
(1) Hexafluoroethane. Source not given. Stated to be manufacturer's research grade, dried over $CaCl_2$ before use.
(2) Perfluorotributylamine. Minnesota Mining and Manufacturing Co. Distilled, used portion boiling between 447.85–448.64 K which gave a single GLC peak. Density at 298.15 K, $\rho = 1.880$ g cm^{-3}.

Estimated Error:
$\delta x_1/x_1 = \pm 0.002$
δN/cal K^{-1} mol^{-1} = ±0.1

References:
[1]J. H. Diamond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

3.10. Pentafluoroethane

Components:
(1) Pentafluoroethane; C_2HF_5; [354-33-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. F. M. Alexander, A. G. M. Abel, and I. M. A. Fonseca, Fluid Phase Eq. **173**, 97–107 (2000).

Variables:
T/K = 289.16–303.03
P_1/Pa = 101 325

Prepared By:
H. L. Clever

Experimental Values

Solubility of pentafluoroethane in water from 289.16 K to 303.03 K.
Mole fraction and Ostwald coefficients at a pressure of 101 325 Pa.

T/K	Mole fraction $10^4 x_1$	Ostwald coefficient ($L_{1,2}$/cm^{3}cm^{-3})	Henry's constant (H_1/MPa)
289.16	7.691	0.996	131.7
290.13	7.639	0.992	132.6
291.03	7.539	0.982	134.4
292.09	7.153	0.935	141.7
293.14	6.943	0.911	145.9
294.20	6.686	0.881	151.6
294.99	6.430	0.849	157.6
296.15	6.300	0.835	160.8
297.34	5.832	0.776	173.7
299.16	5.570	0.746	181.9
299.94	5.344	0.717	189.6
301.23	5.045	0.680	200.8
302.01	4.852	0.656	208.8
303.03	4.704	0.638	215.4

The authors fitted the mole fraction solubility to the equation: $R \ln x_1 = -153.287 + 27\,180.1/(T/\mathrm{K})$ from which they obtained ΔH/J mol^{-1} = −27 180 and ΔS/J K^{-1} mol^{-1} = −153.29. (Reversed values in paper's Table 5.)

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and technique were given in detail in an earlier publication.[1] See methyl fluoride+alcohol data sheets earlier in this volume. The principle of the method is to bring a measured volume of degassed water into contact with a known volume of gas at a given temperature and pressure. After equilibrium is attained the change in volume gives the amount of gas dissolved and the solubility. The method was tested by measuring the solubility of oxygen and of carbon dioxide in water. The results agreed with literature values to ±2%.

Source and Purity of Materials:
(1) Pentafluoromethane or HFC-125. Linde Gas. Purity stated to be 99.9 mol %.
(2) Water. Purified. Degassed by vacuum sublimation technique.

Estimated Error:
δT/K = ±0.01
δp/mmHg = ±0.01
$\delta x_1/x_1 = \pm 0.02$

References:
[1]C. S. O. Silva, I. M. A. Fonseca, and L. Q. Lobo, Fluid Phase Eq. **135**, 137 (1997).

Components:
(1) 1,1,1,2,2-Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 293.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

Solubility of pentafluoroethane in hexadecane between 293.15 K and 363.15 K

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution γ^{∞}
293.15	7.01	7.51
303.15	7.93	6.86
323.15	9.73	5.96
343.15	11.42	–
363.15	12.96	-

Henry's constant: $He/\mathrm{MPa} = \lim_{x_1 \to 0}(f_1/\mathrm{MPa})/x_1$

Isochoric Method. At equilibrium, $f_1^l = f_1^v = \varphi_1^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1^{\infty} = (He_{1,2})/f_1^{*l}$. It is not derived for the solute at temperatures above the critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Melzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1,1,2,2-Pentafluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Hexadecane. Lancaster Synthesis, Morecame, England. Stated to be 99% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
δHe/He = $< \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1,2,2-Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) 2,6,10,14-Tetramethylpentadecane; $C_{19}H_{40}$; [1921-70-6]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 293.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of pentafluoroethane in 2,6,10,14-tetra-methylpentadecane between 293.15 K and 363.15 K

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution γ^{∞}
293.15	5.19	5.55
303.15	5.92	5.12
323.15	7.44	4.55
343.15	8.98	—
363.15	10.49	—

Henry's constant: $He/\mathrm{MPa} = \lim_{x_1 \to 0}(f_1/\mathrm{MPa})/x_1$

Isochoric Method. At equilibrium, $f_1^l = f_1^v = \varphi_1^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1^{\infty} = (He_{1,2})/f^{*l}{}_1$. It is not derived for the solute at temperatures above the critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1,1,2,2-Pentafluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) 2,6,10,14-Tetramethylpentadecane, Sigma Chemical Co., St. Louis, MO. Stated to be of 98% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1,2,2-Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Eicosane; $C_{20}H_{42}$; [112-95-8]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 323.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of pentafluoroethane in eicosane between 323.15 K and 363.15 K

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution γ^{∞}
323.15	9.21	5.63
342.15	10.79	—
363.15	12.24	—

Henry's constant: $He/\text{MPa} = \lim_{x_1 \to 0}(f_1/\text{MPa})/x_1$

Isochoric Method. At equilibrium, $f_1^l = f_1^v = \varphi_1^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1^{\infty} = (He_{1,2})/f^{*l}_1$. It is not derived for the solute at temperatures above the critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1,1,2,2-Pentafluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Eicosane. Sigma Chemical Co., St. Louis, MO. Stated to be 99% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.07–313.18
p_t/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of pentafluoroethane in methanol between 283.07 K and 313.18 K

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant $[H_{1,2}/\text{MPa} = (p_1/\text{MPa})/x_1]$
283.07	0.0318	0.9235	2.94
293.05	0.0238	0.8695	3.69
303.14	0.0169	0.7797	4.66
313.18	0.0107	0.6466	6.12

The authors approximated the pentafluoroethane partial pressure as $p_1/\text{MPa} = (p_t/\text{MPa})y_1 = 0.1013 y_1$.

They fitted the Henry's constants to the equation: $\ln(H_{1,2}/\text{MPa}) = -215.617 + 7822.205/(T/\text{K}) + 33.489 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions.
Measurements were repeated three times.

Source and Purity of Materials:
(1) Pentafluoroethane. Daikin Industries, Ltd. Stated to be greater than 99.8% pure.
(2) Methanol. Wake Pure Chemials, Ltd. Stated to be 99.8% pure.

Estimated Error:
$\delta T/\text{K} = \pm 0.1$
$\delta x_1/x_1 = < \pm 0.02$ for the liquid phase
$= \pm 0.005$ for the vapor phase.
$\delta H/H = \pm 0.025$.

Components:
(1) Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
R. Kato and H. Nishiumi, J. Chem. Eng. Data **47**, 1140–1144 (2002).

Variables:
T/K = 303.0–323.0
p/kPa = 52.1–112.0

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of pentafluoroethane in methanol from 303.0 K to 323.0 K

T/K	p/kPa	Liquid Mol Fraction x_1	Vapor Mol Fraction y_1	Henry's Constant (H/MPa)
303.0	59.4	0.00790	0.613	4.64
	52.1	0.00650	0.564	
	53.1	0.00650	0.571	
308.0	72.7	0.00780	0.574	6.93
	71.7	0.00770	0.579	
	63.6	0.00620	0.522	
	64.1	0.00620	0.526	
313.0	99.4	0.00750	0.518	7.88
	98.4	0.00770	0.525	
	88.1	0.00620	0.473	
	88.7	0.00620	0.473	
323.0	112.0	0.00600	0.462	
	110.0	0.00570	0.447	

The authors fit the Henry constants to the equation $\ln(H/\text{MPa}) = 33.78 - 4146/(T/\text{K}) - 3.253 \ln(T/\text{K})$.
At 303 K and 101 kPa the mole fraction of C_2HF_5 in methanol is 0.0220 and the entropy of solution is $-83.51\ \text{J K}^{-1}\ \text{mol}^{-1}$.

Auxiliary Information

Method/Apparatus/Procedure:
The method was head space gas chromatography. The HS-40 Perkin-Elmer head space autosampler gas chromatograph was used. Equilibrium cells were 22 mL glass vials. The autosampler, in a constant temperature bath, could contain up to 13 vials. The solvent was weighed in a glass ampule and placed in a sample vial; the fluorocarbon was charged into the vial and weighed. The fluorocarbon weight and the air weight replaced by fluorocarbon were used to determine the overall composition. The solvent ampule was broken and the system equilibrated for 3 h, the headspace vapor was injected for 3 s into the gas chromatograph by the auto-sampler program. Details of the calculation are in the paper.

Source and Purity of Material:
(1) Pentafluoroethane. Toei Chem. Ind. (Tokyo). Purity stated to be 99.9%, used as received.
(2) Methanol. Kanto Chem. Ind. (Tokyo). Purity stated to be 99.5%, used as received.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.008 av.; ±0.022 max.
$\delta y_1/y_1$ = ±0.008 av.; ±0.021 max.

Components:
(1) Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.02–313.11
p_t/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of pentafluoroethane in ethanol from 283.02 K to 313.11 K at a partial pressure of 0.1013 MPa

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant [$H_{1,2}$/MPa = (p_1/MPa)/x_1]
283.02	0.0394	0.9697	2.49
292.94	0.0289	0.9429	3.30
303.15	0.0212	0.8961	4.29
313.11	0.0157	0.8258	5.31

The authors approximated the pentafluoroethane partial pressure as $p_1/\text{MPa} = (p_t/\text{MPa})y_1 = 0.1013 y_1$.
They fitted the Henry's constants to the equation: $\ln(H_{1,2}/\text{MPa}) = 110.72 - 6763.19/(T/\text{K}) - 15.218 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions.
Measurements were repeated three times.

Source and Purity of Material:
(1) Pentafluoroethane. Daikin Industries, Ltd. Stated to be greater than 99.8% pure.
(2) Ethanol. Wake Pure Chemicals, Ltd. Stated to be 99.8% pure.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = < ±0.02 for the liquid phase
= ±0.005 for the vapor phase.
$\delta H/H$ = ±0.025.

Components:
(1) Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
R. Kato and H. Nishiumi, J. Chem. Eng. Data **47**, 1140–1144 (2002).

Variables:
T/K = 308.0, 313.0, and 323.0
p/kPa = 54.7–89.1

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of pentafluoroethane in ethanol from 303.0 K to 323.0 K

T/K	p/kPa	Liquid Mol Fraction x_1	Vapor Mol Fraction y_1	Henry's Constant (H/MPa)
303.0	64.5	0.01170	0.752	4.13
	54.7	0.00940	0.711	
	56.5	0.00990	0.719	
313.0	67.8	0.00990	0.712	4.85
	59.8	0.00850	0.682	
323.0	89.1	0.00950	0.640	5.98
	80.5	0.00830	0.613	

The authors fit the Henry constants to the equation $\ln(H/\text{MPa}) = 32.92 - 3519/(T/\text{K}) - 3.501 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
The method was head space gas chromatography. The HS-40 Perkin-Elmer head space autosampler gas chromatograph was used. Equilibrium cells were 22 mL glass vials. The autosampler, in a constant temperature bath, could contain up to 13 vials. The solvent was weighed in a glass ampule and placed in a sample vial; the fluorocarbon was charged into the vial and weighed. The fluorocarbon weight and the air weight replaced by fluorocarbon were used to determine the overall composition. The solvent ampule was broken and the system equilibrated for 3 h, the headspace vapor was injected for 3 s into the gas chromatograph by the auto-sampler program. Details of the calculation are in the paper.

Source and Purity of Material:
(1) Pentafluoroethane. Toei Chem. Ind. (Tokyo). Purity stated to be 99.9%, used as received.
(2) Ethanol. Kanto Chem. Ind. (Tokyo). Purity stated to be 99.5%, used as received.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.008 av.; ±0.022 max.
$\delta y_1/y_1$ = ±0.008 av.; ±0.021 max.

Components:
(1) Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) 2-Propanol; C_3H_8O; [67-63-0]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.16–313.26
p_t/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of pentafluoroethane in 2-propanol from 283.16 K to 313.26 K

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant [$H_{1,2}$/MPa = (p_1/MPa)/x_1]
283.16	0.0376	0.9747	2.62
292.99	0.0293	0.9556	3.30
303.17	0.0230	0.9223	4.05
313.26	0.0179	0.8602	4.87

The authors approximated the pentafluoroethane partial pressure as $p_1/\text{MPa} = (p_t/\text{MPa})y_1 = 0.1013y_1$.
They fitted the Henry's constants to the equation: $\ln(H_{1,2}/\text{MPa}) = 73.392 - 4754.616/(T/\text{K}) - 9.854 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions.
Measurements were repeated three times.

Source and Purity of Material:
(1) Pentafluoroethane. Daikin Industries, Ltd. Stated to be greater than 99.8% pure.
(2) 2-Propanol. Wake Pure Chemicals, Ltd. Stated to be 99.5% pure.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = < ±0.02 for the liquid phase
= ±0.005 for the vapor phase.
$\delta H/H$ = ±0.025.

Components:
(1) Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Pentaerythitol tetrapentanonate ester; $C_{25}H_{44}O_8$; [15834-04-5] *Chem. Abstr.* name: Pentanoic 2,2-*bis*[(1-oxypentyl)oxylmethyl]-1,3-propanediyl ester.

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823–828 (1999).

Variables:
T/K = 303.15–363.15
p_1 /MPa = 0.05–1.9

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1MPa	Mol Fraction x_1
303.15	0.0731	0.0675	343.16	0.1119	0.0444
303.16	0.0991	0.0896	343.17	0.1525	0.0587
303.14	0.1372	0.1265	343.15	0.2139	0.0841
303.16	0.2590	0.2222	343.15	0.6055	0.2238
303.14	0.3688	0.3163	343.15	0.8740	0.3062
303.15	0.5309	0.4208	343.16	1.1990	0.4004
303.15	0.6858	0.5206	343.16	1.6970	0.5192
303.15	0.9926	0.6805			
323.27	0.0936	0.0551	363.17	0.1268	0.0363
323.26	0.1281	0.0725	363.23	0.1732	0.0475
323.26	0.1787	0.1033	363.26	0.2437	0.0684
323.29	0.3385	0.1823	363.28	0.6931	0.1862
323.26	0.4953	0.2687	363.27	0.9985	0.2563
323.26	0.7169	0.3627	363.16	1.3860	0.3414
323.27	0.9611	0.4627	363.25	1.8970	0.4317
323.27	1.3920	0.6141			

Henry's constant was calculated for the 12 points at pressures below 0.25 MPa and fitted to the equation: $\ln(He_{1,2}/\mathrm{MPa}) = \ln(2.050 \pm 0.023) - (2167 \pm 56)[1/(T/\mathrm{K}) - 1/333.15]$. The C_2HF_5 activity coefficients at infinite dilution are: $(T/\mathrm{K})/\gamma^{\infty}$ 303.2/0.93; 323.2/1.04.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from pressure changes in a gas system of known volume, observed during the absorption of the gas. The apparatus consists of three sections. (*i*) A liquid bath thermostat 1 containing the equilibrium cell with a magnetic stirrer; (*ii*) liquid bath thermostat 2 with a gas bottle of calibrated volume; (*iii*) an air bath thermostat with a pressure transmitter and connections between the first two sections and to a gas storage and a vacuum pump. More details of the apparatus, the experimental technique, and the treatment of the data are in an earlier paper of the authors.[1]

Source and Purity of Material:
(1) Pentafluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Pentaerythritol tetrapentanonate ester. Synthesized[2] by a reaction between valeric acid and pentaerythirtol catalyzed with p-toluenesulfonic acid in a p-xylene solvent. The product was vacuum distilled. NMR and IR results gave a purity >95%.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p_1/p_1 = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressures,
$= < \pm 0.03$ at high pressures.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]K. D. Black and F. D. Gunstone, Chem. Phys. Lipids **56**, 169 (1990).

Components:
(1) 1,1,1,2,2-Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Pentaerythritol tetra-2-ethylbutanoate; $C_{29}H_{52}O_8$; [139116-32-8]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 323.08–363.25
p_1 /MPa = 0.1651–1.9669

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1 /MPa	Mol Fraction x_1
303.15	The Solvent is a solid at this temperature		343.25	0.1658	0.0750
			343.19	0.1819	0.0820
			343.24	0.2019	0.0913
			343.22	0.4858	0.1985
			343.24	0.9374	0.3598
323.11	0.1404	0.0817	343.22	1.1996	0.4321
323.04	0.1519	0.1024	343.25	1.5109	0.5149
323.07	0.1686	0.1112			
323.09	0.4006	0.2243	363.28	0.1868	0.0603
323.09	0.7709	0.3807	363.23	0.2058	0.0665
323.11	0.9592	0.4548	363.21	0.22281	0.0744
323.11	1.2094	0.5716	363.24	0.5534	0.1615
			363.22	1.0590	0.2996
			363.24	1.3842	0.3666
			363.27	1.7228	0.4385

$\ln(H_{2,1}/\mathrm{MPa}) = (1.779 \pm 0.012) - (2119 \pm 42)[1/(T/\mathrm{K}) - 1/333.15]$.
Solvent Chem. Abstr. Name: 2,2-bis[(2-ethyl-1-oxybutoxy)methyl]-1,3-propanediyl ester of 2ethylbutanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) 1,1,1,2,2-Pentafluoroethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylbutanoate. Synthesized from pentaerythriol and 2-ethyl-butanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%. Melting point 310–312 K.

Estimated Error:
Uncertanties in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) 1,1,1,2,2-Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Pentaerythritol tetra-2-ethylhexanoate; $C_{37}H_{68}O_8$; [7299-99-2]—C.A. name below.

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 303.11–363.29
p_1 /MPa = 0.1322–1.8071

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mole Fraction x_1	T/K	p_1 /MPa	Mole Fraction x_1
303.11	0.1322	0.1321	343.22	0.1880	0.0846
303.11	0.1508	0.1468	343.20	0.2138	0.0943
303.14	0.1605	0.1577	343.24	0.2286	0.1019
303.16	0.4732	0.4003	343.16	0.7314	0.2951
303.15	0.7054	0.5314	343.17	1.1890	0.4109
303.15	1.0272	0.6812	343.16	1.6389	0.5208
323.07	0.1620	0.1066	363.21	0.2075	0.0689
323.04	0.1841	0.1190	363.15	0.2368	0.0759
323.08	0.1973	0.1275	363.20	0.2527	0.0829
323.26	0.6157	0.3446	363.26	0.8208	0.2544
323.26	0.9660	0.4724	363.29	1.3647	0.3514
323.25	1.3836	0.6048	363.23	1.8071	0.4393

$\ln(H_{1,2}/\text{MPa}) = (1.805 \pm 0.014) - (2027 \pm 37)[1/(T/\text{K}) - 1/333.15]$.

Solvent Chem. Abstr. Name: 2,2-bis[(2-ethyl-1-oxyhexyl)oxylmethyl]-1,3-propanediyl ester of 2-ethyl hexanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) 1,1,1,22-Pentafluoroethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylhexanoate. Synthesized from pentaerythriiol and 2-ethyl-hexanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >90%. Contains 5%–10% di- and tri-esters.

Estimated Error:
Uncertanies in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) 1,1,1,2,2-Pentafluoroethane or HFC125; C_2HF_5; [354-33-6]
(2) Pentaerythritol tetrananoate; $C_{41}H_{76}O_8$; [14450-05-6]—C. A. Name below table.

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 302.88–363.33
p_1 /MPa = 0.0928–2.1035

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mole Fraction x_1	T/K	p_1 /MPa	Mole Fraction x_1
303.15	0.0928	0.0787	343.25	0.1295	0.0532
302.91	0.1021	0.0867	343.23	0.1422	0.0592
303.11	0.2462	0.2033	343.20	0.3093	0.1225
302.91	0.3729	0.2861	343.23	0.5168	0.1924
302.91	0.4993	0.3611	343.23	0.6556	0.2365
302.88	0.9493	0.5715	343.23	1.4358	0.4333
302.88	1.2951	0.6985	343.24	1.9431	0.5328
323.09	0.1115	0.0656	363.22	0.1442	0.0435
323.08	0.1226	0.0725	363.33	0.1579	0.0489
323.05	0.2826	0.1569	363.16	0.3290	0.0972
323.08	0.4537	0.2345	363.32	0.5651	0.1593
323.08	0.5913	0.2913	363.32	0.7018	0.1927
323.07	1.2093	0.4919	363.27	1.5910	0.3736
323.08	1.6548	0.6017	363.28	2.1035	0.4582

$\ln(H_{2,1}/\text{MPa}) = (2.015 \pm 0.014) - (1568 \pm 39)[1/(T/\text{K}) - 1/333.15]$.

Solvent Chem. Abstr. Name: 2,2-bis[(1-oxononyl)oxylmethyl]-1,3-propanediyl ester of nonanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) 1,1,1,2,2-Pentafluoroethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetranonanoate. Synthesized from pentaerythriiol and nonanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled.
NMR and IR gave a purity of >95%.

Estimated Error:
Uncertanies in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling J. Chem. Eng. Data **44**, 823 (1999).

Components:

(1) Pentafluoroethane or HFC-125; C_2HF_5; [354-33-6]
(2) Polyol ester mixture; $C(CH_2OOCR)_4$ with R of $n=5\sim10$.

Original Measurements:

Y. Takaishi, M. Izumi, and K. Oguchi, Int. Conf. CFC's, The Day After, IIR/IIF: pp. 99–105, 1994; *Sci. Tech. Froid.* (2 CFCs, the day after) 99–105 (1994).

Variables:

T/K=263.15–313.15
p/MPa=0.228–2.007

Prepared By:

H. L. Clever

Experimental Values

Temperature T/K	Pressure p_1/MPa	Weight Fraction w_1	Mole Fraction x_1	Activity Coefficient γ_1
263.15	0.483	1.000	1.000	1.000
	0.475	0.900	0.979	1.006
	0.470	0.838	0.963	1.014
	0.461	0.727	0.931	1.031
	0.446	0.635	0.898	1.038
	0.415	0.530	0.851	1.027
	0.386	0.459	0.812	1.008
	0.319	0.343	0.735	0.935
	0.232	0.240	0.616	0.828
	0.228	0.231	0.604	0.831
273.15	0.671	1.000	1.000	1.000
	0.658	0.899	0.978	1.006
	0.651	0.837	0.963	1.012
	0.640	0.724	0.930	1.033
	0.618	0.632	0.897	1.039
	0.579	0.526	0.849	1.038
	0.537	0.455	0.809	1.019
	0.444	0.349	0.732	0.950
	0.329	0.236	0.611	0.864
	0.320	0.228	0.600	0.858
283.15	0.909	1.000	1.000	1.000
	0.890	0.898	0.978	1.005
	0.881	0.835	0.963	1.012
	0.865	0.722	0.930	1.033
	0.839	0.628	0.896	1.045
	0.786	0.521	0.847	1.047
	0.727	0.450	0.806	1.029
	0.607	0.344	0.727	0.975
	0.447	0.231	0.604	0.891
	0.435	0.224	0.595	0.882
293.15	1.205	1.000	1.000	1.000
	1.180	0.896	0.978	1.006
	1.167	0.832	0.962	1.014
	1.147	0.718	0.928	1.037
	1.109	0.622	0.893	1.049
	1.039	0.515	0.844	1.053
	0.962	0.443	0.802	1.041
	0.798	0.338	0.722	0.987
	0.585	0.226	0.597	0.907
	0.571	0.219	0.588	0.901
303.15	1.568	1.000	1.000	1.000
	1.533	0.894	0.977	1.007
	1.518	0.829	0.961	1.016
	1.494	0.712	0.926	1.042
	1.448	0.615	0.890	1.059
	1.348	0.506	0.839	1.063
	1.243	0.435	0.797	1.050
	1.032	0.330	0.715	1.005
	0.747	0.221	0.591	0.919
	0.731	0.214	0.581	0.917
313.15	2.007	1.000	1.000	1.000
	1.961	0.891	0.977	1.007
	1.944	0.824	0.960	1.019
	1.917	0.704	0.924	1.048
	1.853	0.603	0.885	1.069
	1.713	0.494	0.832	1.074
	1.570	0.424	0.789	1.061
	1.293	0.321	0.706	1.016
	0.928	0.214	0.581	0.932
	0.910	0.208	0.572	0.931

Auxiliary Information

Method/Apparatus/Procedure:

The experimental apparatus consists of glass equilibrium cell of volume 17.93 cm^3, a temperature measuring system and a pressure measuring system. It is described in detail in an earlier paper.[1] The HFC-125 is completely miscible with the polyol ester at all temperatures and pressures of this study. The activity coefficients from the data show little dependence on temperature. It is assumed that only the HFC-125 occurs in the vapor space. Equations for the correlation of system solubility by a vapor-liquid equilibrium calculation are given. The authors show a figure of pressure vs weight fraction HFC-125 +naphthenic oil[2] which shows two phase immiscibility starting at less than 0.2 weight fraction HFC-125 at temperatures from 273.15 K to 313.15 K.

Source and Purity of Material:

(1) Pentafluoroethane. Du Pont-Mitsui Fluorochemicals Co., Ltd., Tokyo. Purity not specified.
(2) Polyol ester lubricating oil. Kyodo Oil Technical Research Center Co., Ltd., Saitama Japan. Mol wt 610; Kinematic viscosity is 31 $mm^2\ s^{-1}$ at 313.15 K.

Estimated Error:

δT/K=±0.010
δp/kPa=±2
$\delta w_1/w_1$=±0.005

References:

[1]Y. Takaishi and K. Oguchi, Trans. JAR **7**, 75–84 (1990).
[2]Y. Tanaka *et al.* Proc. 2nd Asian Thermophys. Properties Conference, 375 (1989).

3.11. 1,1,1,2-Tetrafluoroethane

Components:
(1) 1,1,1,2-Tetrafluoroethane; $C_2H_2F_4$; [811-97-2]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
D.-Q. Zheng, T.-M. Guo, and H. Knapp, Fluid Phase Eq. **129**, 197–209 (1997).

Variables:
T/K = 278.16–338.17
p/MPa = 0.06093–0.09436

Prepared By:
H. L. Clever

Experimental Values

Solubility of $C_2H_2F_4$ in water and aqueous NaCl

T/K	p/MPa	Sodium Chloride (n_2 /mol mol^{-1})	Mole Fraction $10^4 x_1$	Henry's Constant ($H_{1,s}$ /MPa)
278.16	0.06093	0.00	3.82	154.8
278.16	0.06377		4.08	152.0
308.08	0.07976		1.61	453.6
308.08	0.08302		1.68	453.7
338.12	0.09025		0.782	822.6
338.12	0.09306		0.812	837.3
278.17	0.06753	0.0121	3.58	178.1
278.17	0.08557		3.75	175.0
308.16	0.08216		1.43	526.9
308.16	0.08446		1.50	519.5
338.04	0.09212		0.683	973.6
338.04	0.09403		0.700	975.9
278.15	0.06694	0.0295	2.84	229.3
278.15	0.07008		3.01	225.8
308.16	0.08076		1.16	639.5
308.16	0.08084		1.19	623.6
338.14	0.08978		0.548	1178.
338.14	0.08979		0.562	1148.
278.16	0.07033	0.0564	2.02	338.8
278.16	0.07524		2.16	338.4
308.20	0.08434		0.693	1122.
308.20	0.08719		0.730	1104.
338.17	0.08931		0.274	2368.
338.17	0.09436		0.279	2588.

The above NaCl mol ratios correspond to 0.672, 1.64 and 3.13 mol kg^{-1} (molality), respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental apparatus consists of a degassing system and a gas absorption unit. The water and NaCl solutions were degassed by vacuum with stirring until the vapor pressure of the solvent was reached. The degassed solvent was transferred to an evacuated glass cell and weighed to 0.0001 g. The cell was thermostated and the adsorption apparatus evacuated before the gas was admitted. The solvent was stirred constantly. When the system T and p were constant, the equilibrium state was established.

Source and Purity of Material:
(1) 1,1,1,2-Tetrafluoroethane or R-134a. Hoechst. Purity stated to be 99.5 volume %.
(2) Sodium chloride. Merck. Laboratory grade.
(3) Water. Deionized at the Institute.

Estimated Error:
δT/K = ±0.1
$\delta p/p$ = ±0.001
$\delta x_1/x_1$ = ±0.005
(Compiler's estimates).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Tridecane; $C_{13}H_{28}$; [629-50-5]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 303.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane in tridecane from 303.15 K to 363.15 K

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution (γ^∞)
303.15	4.11	6.36
323.15	5.44	5.31
343.15	6.79	4.58
363.15	8.18	4.13

Henry's constant He/MPa = $\lim_{x_1 \to 0}(f_1$ /MPa$)/x_1$

Isochoric Method. At equilibrium $f_1^l = f_1^v = \varphi_1^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1^\infty = (He_{1,2})/f^{*l}_1$. Not derived for temperatures of the solute when it is above its critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Material:
(1) 1,1,1,2-Tetrafluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Tridecane. Sigma Chemical Co., St. Louis, MO. Stated to be 99% pure.

Estimated Error:
$\delta T/T$ = ±0.00016
$\delta p/p$ = ±0.001
$\delta He/He$ = < ±0.02 at low pressure;
= < ±0.03 at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. 75, 544–550 (1997).

Variables:
T/K = 293.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane in hexadecane from 293.15 K to 363.15 K

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution γ^{∞}
293.15	3.52	7.11
303.15	4.10	6.34
323.15	5.32	5.21
343.15	6.58	4.45
363.15	7.83	3.96

Henry's constant: $He/\mathrm{MPa} = \lim_{x_1 \to 0}(f_1/\mathrm{MPa})/x_1$

Isochoric Method. At equilibrium $f_1{}^l = f_1{}^v = \varphi_1{}^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1{}^{\infty} = (He_{1,2})/f^{*l}{}_1$. Not derived for temperatures of the solute when it is above its critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Hexadecane. Lancaster Synthesis. Stated to be 99% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) 2,6,10,14-Tetramethylpentadecane; $C_{19}H_{40}$; [1921-70-6]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 293.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane in 2,6,10,14-tetramethylpentane from 293.15 K to 363.15 K

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution γ^{∞}
293.15	2.64	5.35
303.15	3.15	4.86
323.15	4.21	4.12
343.15	5.33	3.61
363.15	6.51	3.29

Henry's constant: $He/\mathrm{MPa} = \lim_{x_1 \to 0}(f_1/\mathrm{MPa})/x_1$

Isochoric Method. At equilibrium $f_1{}^l = f_1{}^v = \varphi_1{}^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1{}^{\infty} = (He_{1,2})/f^{*l}{}_1$. Not derived for temperatures of the solute when it is above its critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) 2,6,10,14-Tetramethylpenadecane. Sigma Chemical Co., St. Louis, MO. Stated to be of 98% pure.

Estimated Error:
$\delta p/p = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Eicosane; $C_{20}H_{42}$; [112-95-8]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 323.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane in eicosane from 323.15 to 363.15K

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution γ^{α}
323.15	5.04	4.92
343.15	6.28	4.24
363.15	7.38	3.82

Henry's constant: $He/\text{MPa} = \lim_{x_1 \to 0}(f_1/\text{MPa})/x_1$

Isochoric Method. At equilibrium $f_1{}^l = f_1{}^v = \varphi_1{}^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1{}^{\infty} = (He_{1,2})/f^{*l}{}_1$. Not derived for temperatures of the solute when it is above its critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2)Eicosane. Sigma Chemical Co., St. Louis, MO. Stated to be 99% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Methanol; CH_4O; [65-56-1]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.26–313.08
p_t /MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane in methanol from 283.26 K to 313.08 K.

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant $[H_{1,2}/\text{MPa} = (p_1/\text{MPa})/x_1]$
283.26	0.0629	0.9309	1.49
293.04	0.426	0.8761	2.08
302.93	0.0287	0.7822	2.75
313.08	0.0176	0.6546	3.77

The authors approximated the 1,1,1,2-tetrafluoroethane partial pressure as $p_1/\text{MPa} = (p_t/\text{MPa})/y_1) = 0.1013 y_1$.

They fitted the Henry's constants to the equation: $\ln(H_{1,2}/\text{MPa}) = -29.597 - 960.938/(T/\text{K}) + 5.915 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions. Measurements were repeated three times.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. Daikin Industries, Ltd. Stated to be greater than 99.8% pure.
(2) Methanol. Wake Pure Chemicals, Ltd. Stated to be 99.8% pure.

Estimated Error:
$\delta T/\text{K} = \pm 0.1$
$\delta x_1/x_1 = < \pm 0.02$ for the liquid phase.
$= \pm 0.005$ for the vapor phase.
$\delta H/H = \pm 0.025$.

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
R. Kato and H. Nishiumi, J. Chem. Eng. Data **47**, 1140–1144 (2002).

Variables:
T/K = 303.0–323.0
p/kPa = 42.4–92.9

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane in methanol from 303.0 K to 323.0 K

T/K	p/kPa	Liquid Mol Fraction x_1	Vapor Mol Fraction y_1	Henry's Constant (H/MPa)
303.0	50.6	0.01070	0.549	2.58
	49.6	0.01040	0.542	
	42.4	0.00800	0.480	
308.0	60.9	0.01000	0.498	3.05
	54.3	0.00780	0.442	
313.0	70.5	0.00980	0.473	3.41
	70.4	0.00960	0.471	
	47.0	0.00750	0.535	
323.0	92.9	0.00740	0.388	4.88
	85.6	0.00590	0.328	

The authors fit the Henry constants to the equation $\ln(H/\text{MPa}) = 33.41 - 4073/(T/\text{K}) - 3.331 \ln(T/\text{K})$.
At 303 K and 101 kPa the mole fraction of $C_2H_2F_4$ in methanol is 0.0392 and the entropy of solution is 81.00 J K^{-1} mol^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:
The method was head space gas chromatography. The HS-40 Perkin-Elmer head space autosampler gas chromatography was used. Equilibrium cells were 22 mL glass vials. The autosampler, in a constant temperature bath, could contain up to 13 vials. The solvent was weighed in a glass ampule and placed in a sample vial; the fluorocarbon was charged into the vial and weighed. The fluorocarbon weight and the air weight replaced by fluorocarbon were used to determine the overall composition. The solvent ampule was broken and the system equilibrated for 3 h, the headspace vapor was injected for 3 s into the gas chromatograph by the auto-sample program. Details of the calculation are in the paper.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. Toei Chem. Ind. (Tokyo). Purity stated to be 99.9%, used as received.
(2) Methanol. Kanto Chem. Ind. (Tokyo). Purity stated to be 99.5%, used as received.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.008 av.; ±0.022 max.
$\delta y_1/y_1$ = ±0.008 av.; ±0.021 max.

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Ethanol; $C_{19}H_6O$; [64-17-5]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.17–313.13
p_t/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane 283.17 K to 313.13 K

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant [$H_{1,2}$/MPa = (p_1/MPa)/x_1]
283.17	0.0579	0.9702	1.69
293.03	0.0440	0.9444	2.17
303.09	0.0330	0.9003	2.76
313.13	0.0246	0.8230	3.39

The authors approximated the 1,1,1,2-tetrafluoroethane partial pressure as $p_1/\text{MPa} = (p_t/\text{MPa})y_1 = 0.1013y_1$.
They fitted the Henry's constants to the equation: $\ln(H_{1,2}/\text{MPa}) = 56.848 - 4238.572/(T/\text{K}) - 7.324 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions. Measurements were repeated three times.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. Daikin Industries, Ltd. Stated to be greater than 99.8% pure.
(2) Ethanol. Wake Pure Chemicals, Ltd. Stated to be 99.8% pure.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = < ±0.02 for the liquid phase.
= ±0.005 for the vapor phase.
$\delta H/H$ = ±0.025.

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
R. Kato and H. Nishiumi, J. Chem. Eng. Data **47**, 1140–144 (2002).

Variables:
T/K = 303.0–323.0
p/kPa = 35.4–75.4

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane in ethanol from 303.0 K to 323.0 K

T/K	p/kPa	Liquid Mol Fraction x_1	Vapor Mol Fraction y_1	Henry's Constant (H/MPa)
303.0	35.4	0.01020	0.748	2.61
	37.5	0.01090	0.761	
308.0	54.6	0.01340	0.712	2.88
	45.0	0.01050	0.659	
	43.9	0.00990	0.655	
313.0	57.7	0.01230	0.663	3.11
	58.6	0.01250	0.664	
	52.4	0.01080	0.638	
	51.7	0.01060	0.642	
323.0	75.4	0.01040	0.580	4.23
	74.9	0.01010	0.576	

The authors fit the Henry constants to the equation $\ln(H/\text{MPa}) = 32.66 - 3483/(T/\text{K}) - 3.543 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
The method was head space gas chromatography. The HS-40 Perkin-Elmer head space autosampler gas chromatography was used. Equilibrium cells were 22 mL glass vials. The autosampler, in a constant temperature bath, could contain up to 13 vials. The solvent was weighted in a glass ampule and placed in a sample vial; the fluorocarbon was charged into the vial and weighed. The fluorocarbon weight and the air weight replaced by fluorocarbon were used to determine the overall composition. The solvent ampule was broken and the system equilibrated for 3 h, the headspace vapor was injected for 3 s into the gas chromatography by the auto-sample program. Details of the calculation are in the paper.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrathane. Toei Chem. Ind. (Tokyo). Purity stated to be 99.9%, used as received.
(2) Ethanol. Kanto Chem. Ind. (Tokyo). Purity stated to be 99.5%, used as received

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.008 av.; ±0.022 max.
$\delta y_1/y_1$ = ±0.008 av.; ±0.021 max.

Components:
(1) 1,1-Tetrafluoroethane or HFC152a; $C_2H_2F_4$; [811-97-2]
(2) 2-Propanol; C_3H_8O; [67-63-0]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.25–313.25
p_t/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1,1,2-tetrafluoroethane in 2-propanol from 283.25 K to 313.25 K

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant [$H_{1,2}$/MPa = (p_1/MPa)]
283.25	0.0518	0.9799	1.91
293.08	0.0408	0.9603	2.38
303.1	0.0308	0.9205	3.02
313.25	0.0255	0.8617	3.42

The authors approximated the 1,1,2-tetrafluoroethane partial pressure as $p_1/\text{MPa} = (p_t/\text{MPa})y_1 = 0.1013y_1$.
They fitted the Henry's constants to the equation:
$\ln(H_{1,2}/\text{MPa}) = 227.428 - 11\,566.178/(T/\text{K}) - 32.933 \ln(T/\text{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions. Measurements were repeated three times.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. Daikin Industries, Ltd. Stated to be greater than 99.8% pure.
(2) 2-Propanol. Wake Pure Chemicals, Ltd. Stated to be 99.5% pure.

δT/K = ±0.1
$\delta x_1/x_1$ = < ±0.02 for the liquid phase
= ±0.005 for the vapor phase.
$\delta H/H$ = ±0.025.

Components:
(1) 1,1-Tetrafluoroethane or HFC-132a; $C_2H_2F_4$; [811-97-2]
(2) Triethylene glycol dimethyl ether; $C_3H_8O_4$

Original Measurements:
A. Coronas, A. M. Mainar, K. R. Patil, A. Conesa, S. Shen, and S. Zhu, J. Chem. Eng. Data **47**, 56–58 (2002).

Variables:
T/K = 283.25–353.25
p_1 /kPa = 24.89–2203.3

Prepared By:
H. L. Clever

Experimental Values

T/K	Vap Pressure[a] (p_1/kPa)	Mol Fraction x_1	Activity Coefficient γ_1	T/K	Vap Pressure (p_1 /kPa)	Mol Fraction x_1	Activity Coefficient γ_1
283.15	24.89	0.1083	0.6004	323.16	83.76	0.0927	0.7885
	48.33	0.2015	0.6484		186.0	0.1964	0.8185
	75.44	0.2952	0.6993		284.5	0.2890	0.8462
	112.11	0.3982	0.7472		372.2	0.3670	0.8697
	145.7	0.4797	0.8035		476.8	0.4501	0.8945
	174.8	0.5440	0.8394		602.6	0.5410	0.9207
	198.1	0.5937	0.8664		676.2	0.5919	0.9346
	256.1	0.6910	0.9155		821.4	0.6844	0.9578
	311.1	0.7962	0.9597		981.7	0.7898	0.9797
	363.2	0.9031	0.9901		1136.2	0.9004	0.9950
293.15	36.19	0.1052	0.6463	333.15	103.49	0.0887	0.8376
	72.12	0.2005	0.9808[b]		239.4	0.1947	0.8611
	110.40	0.2941	0.7365		365.3	0.2869	0.8822
	160.3	0.3923	0.7857		463.9	0.3562	0.8981
	206.2	0.4742	0.8269		595.5	0.4395	0.9172
	249.0	0.5434	0.8608		772.3	0.5402	0.9394
	281.4	0.5933	0.8845		865.5	0.5915	0.9501
	356.0	0.6897	0.9268		1041.5	0.6822	0.9674
	429.9	0.7950	0.9651		1245.5	0.7874	0.9842
	499.9	0.9026	0.9915		1439.7	0.8995	0.9961
303.15	49.79	0.1016	0.6929	343.15	124.52	0.0840	0.8877
	101.91	0.1994	0.7334		301.4	0.1928	0.9038
	156.6	0.2927	0.7734		459.1	0.2846	0.9180
	219.5	0.3852	0.8138		563.6	0.3446	0.9274
	281.4	0.4675	0.8496		725.8	0.4280	0.9405
	343.5	0.5426	0.8815		969.2	0.5395	0.9575
	387.8	0.5928	0.9018		1087.3	0.5914	0.9650
	491.3	0.6883	0.9376		1296.0	0.6797	0.9768
	578.8	0.7935	0.9702		1547.5	0.7848	0.9886
	671.6	0.9020	0.9927		1794.6	0.8985	0.9972
313.15	65.72	0.0976	0.7403	353.15	146.3	0.0794	0.9388
	140.0	0.1980	0.7759		371.3	0.1908	0.9465
	214.3	0.2910	0.8099		565.2	0.2823	0.9536
	290.4	0.3767	0.8417		669.2	0.3325	0.9577
	371.6	0.4595	0.8721		865.3	0.4157	0.9647
	460.8	0.5419	0.9014		1192.6	0.5392	0.9751
	517.9	0.5923	0.9185		1335.3	0.5917	0.9794
	635.8	0.6865	0.9479		1585.5	0.6775	0.9860
	761.6	0.7918	0.9750		1891.8	0.7822	0.9930
	882.7	0.9013	0.9939		2203.3	0.8976	0.9983

[a]This is the total pressure, but the authors say since that the liquid vapor pressure is so small they assume it is all due to the solute gas.
[b]This the value in the paper, it probably should be 0.6808.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was measured by a static method described previously.[1] The apparatus consists of an equilibrium cell, a double walled 25 L capacity water thermostat, a differential null transducer, a precise pressure controller, and two proportional temperature controllers.

A new high pressure equilibrium cell of 149 cm^3 volume was constructed and used.

An auxiliary stainless steel container was used to prepare the mixture. A known mass of the ether was added to the equilibrium cell and then with a known mass of the HFC-134a through the auxiliary vessel.

The apparatus was tested by measuring the vapor pressure of the HFC-134a. It correlated within 0.28% of accepted value.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. DuPont. Stated to be >99.9% in mass.
(2) Triethylene glycol dimethyl ether. Aldrich. Stated to be 99 +%.

Estimated Error:
δT/K = ±0.001
δp_1 /kPa = ±0.05 for pressures >130 kPa;
±0.3 for pressures up to 1 MPa; and
±0.6 for higher pressures.
δx_1 = ±0.0001

References:
[1]X. Esteves, S. K. Chaudhari, and A. Coronas, J. Chem. Eng. Data **40**, 1252 (1995).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) 2-Pentaerythitol tetrapentanonate ester; $C_{25}H_{44}O_8$; [15834-04-5] *Chem. Abstr.* name: Pentanoic 2,2-*bis*[(1-oxypentyl)oxylmethyl]-1,3-propanediyl ester.

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823–828 (1999).

Variables:
T/K = 303.15–363.15
p_1 /MPa = 0.05–1.9

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1MPa	Mol Fraction x_1
303.14	0.0515	0.0907	343.15	0.0939	0.0662
303.15	0.0902	0.1551	343.16	0.1679	0.1151
303.14	0.1321	0.2219	343.27	0.2254	0.1554
303.15	0.1765	0.2737	343.15	0.3326	0.2095
303.16	0.2727	0.3962	343.16	0.5239	0.3130
303.14	0.3258	0.4593	343.14	0.6451	0.3734
303.15	0.4583	0.5942	343.15	0.8953	0.4760
323.26	0.0731	0.0781	363.24	0.1129	0.0558
323.26	0.1296	0.1348	363.26	0.2031	0.0973
323.11	0.1815	0.1877	363.25	0.2615	0.1275
323.28	0.2556	0.2418	363.19	0.4046	0.1779
323.27	0.3997	0.3562	363.21	0.6350	0.2708
323.26	0.4854	0.4190	363.25	0.7914	0.3264
323.26	0.6835	0.5414	363.26	1.0650	0.4079

Henry's constant was calculated for the 12 points below 0.26 MPa and fitted to the equation $\ln(He_{1,2}/\mathrm{MPa}) = \ln(1.138 \pm 0.011) - (2300 \pm 48)[1/(T/\mathrm{K}) - 1/333.15]$. The CH_2F_2 activity coefficients at infinite dilution are: $(T/\mathrm{K})/\gamma^{\infty}$ 303.2/0.88; 323.2/0.91; 343.2/0.95; 363.2/1.01.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from pressure changes in a gas system of known volume, observed during the absorption of the gas. The apparatus consists of three sections: (*i*) A liquid bath thermostat 1 containing the equilibrium cell with a magnetic stirrer; (*ii*) liquid bath thermostat 2 with a gas bottle calibrated volume; (*iii*) an air bath thermostat with a pressure transmitter and connections between the first two sections and to a gas storage and a vacuum pump. More details of the apparatus, the experimental technique, and the treatment of the data are in an earlier paper of the authors.[1]

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. ICI Chemicals & Polymers, Runcorn, Cheshire, U.K. Stated to be 99.9% pure.
(2) Pentaerythritol tetrapentanonate ester. Synthesized[2] by a reaction between valeric acid and pentaerythirtol catalyzed with p-toluensulfonic acid in a p-xylene solvent. The product was vacuum distilled. NMR and IR results gave a purity>95%.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p_1/p_1 = \pm 0.001$
$\delta He/He = <0.02$ at low pressures,
$= < \pm 0.03$ at high pressures.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]K. D. Black and F. D. Gunstone, Chem. Phys. Lipids **56**, 169 (1990).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Pentaerythritol tetra-2-ethylbutanoate; $C_{29}H_{52}O_8$; [139116-32-8]: C. A. name below.

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 323.25–363.29
p_1 /MPa = 0.1106–1.0126

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1MPa	Mol Fraction x_1	T/K	p_1MPa	Mol Fraction x_1
303.15		0.1106	343.29	0.1406	0.1065
	The	0.1144	343.25	0.1464	0.1105
	solvent	0.1275	343.27	0.1615	0.1232
	is a solid	0.2619	343.28	0.3401	0.2382
	at this	0.4333	343.25	0.5702	0.3552
	temperature	0.4489	343.27	0.5817	0.3652
		0.6320	343.26	0.8401	0.4790
323.13		0.1282	363.29	0.1657	0.0886
323.09		0.1315	363.22	0.1741	0.0923
323.11		0.1466	363.24	0.1909	0.1031
323.11		0.2767	363.24	0.4073	0.2034
323.10		0.4036	363.23	0.6887	0.3082
323.12		0.4178	363.25	0.6914	0.3139
323.11		0.5349	263.24	1.0126	0.4198

$\ln(H_{2,1}/\mathrm{MPa}) = (1.048 \pm 0.009) - (2240 \pm 52)(1/(T/\mathrm{K}) - 1/333.15)$
Solvent Chem. Abstracts Name: 2,2-bis-1,3-propaneidyl ester of 2ethylbutanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in author paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. ICI Chemicals and Polymers Ltd., Runcorn, Cheshire, U.K. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylbutanoate. Synthesized from pentaerythriol and 2-ethylbutanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%. Melting point 312–312 K.

Estimated Error:
Uncertanies in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem Eng. **75**, 544 (1997).
[2]J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Pentaerythritol tetra-2-ethylhexanoate; $C_{37}H_{68}O_8$; [7299-99-2]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 303.13–363.24
p_1 /MPa = 0.0873–1.2047

Prepared By:
H. L. Clever

Experimental Values

The solubility of 1,1,1,2-tetrafluoroethane in pentaerythritol tetra-2-ethylhexanoate from 303.13 to 363.24 K

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1MPa	Mol Fraction x_1
303.14	0.0901	0.1515	343.15	0.1080	0.0791
303.16	0.1110	0.1881	343.26	0.1453	0.1043
303.14	0.2142	0.3244	343.12	0.1903	0.1357
303.13	0.3224	0.4475	343.15	0.3841	0.2529
303.16	0.5389	0.6530	343.13	0.5871	0.3533
			343.15	1.0257	0.5334
323.24	0.0873	0.0941	363.22	0.1269	0.0653
323.09	0.1183	0.1275	363.21	0.1675	0.0855
323.24	0.1521	0.1610	363.23	0.2243	0.1133
323.24	0.3007	0.2895	363.24	0.4607	0.2191
323.23	0.4580	0.4022	363.23	0.6999	0.3057
323.25	0.7952	0.5997	363.22	1.2047	0.4637

$\ln(H_{2,1}/\text{MPa}) = (1.112 \pm 0.005) - (2193 \pm 24)[1/(T/\text{K}) - 1/333.15]$

Solvent: Chem. Abstracts Name: 2,2-bis[(2-ethyl-1-oxyhexyl)oxyhexyl)oxylmethyl]-1,3-propanediyl ester of 2-ethyl hexanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at inifinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. ICI Chemicals and Polymers, Ltd., Runcorn, Cheshire, U.K. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylhexanoate. Synthesized from pentaerythriiol and 2-ethlyhexanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >90%. Contains 5%–10% di- and tri-esters.

Estimated Error:
Uncertanties in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC134a; $C_2H_2F_4$; [811-97-2]
(2) Pentaerythritol tetrananoate; $C_{41}H_{76}O_8$; [14450-05-6]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 302.90–363.33
p_1 /MPa = 0.1038–1.2183

Prepared By:
H. L. Clever

Experimental Values

The solubility of 1,1,1,2-tetrafluoroethane in pentaerythritol tetrananoate from 302.90 to 363.33 K.

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1MPa	Mol Fraction x_1
303.15	0.1038	0.1622	343.25	0.1630	0.1138
303.14	0.1186	0.1843	343.26	0.1806	0.1269
303.16	0.1677	0.2499	343.25	0.2387	0.1629
303.14	0.3326	0.4146	343.24	0.5558	0.3143
302.90	0.4160	0.4917	343.23	0.7163	0.3852
302.91	0.4743	0.5399	343.23	0.7811	0.4067
302.90	0.6056	0.6480	343.23	1.0700	0.5155
323.09	0.1348	0.1370	363.22	0.1863	0.0949
323.11	0.1514	0.1542	363.24	0.2035	0.1060
323.10	0.2071	0.2031	363.22	0.2622	0.1322
323.09	0.4503	0.3646	363.23	0.6417	0.2696
323.07	0.5746	0.4395	363.33	0.8312	0.3355
323.07	0.6433	0.4749	363.31	0.8830	0.3450
323.07	0.8616	0.5864	363.31	1.2183	0.4482

$\ln(H_{2,1}/\text{MPa}) = (1.155 \pm 0.011) - (2017 \pm 47)[1/(T/\text{K}) - 1/333.15]$

Solvent Chem. Abstr. Name: 2,2-bis[(1-oxononyl)oxylmethyl1]-1,3-propanediyl ester of nonanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. ICI Chemicals and Polymers, Ltd., Runcorn, Cheshire, U.K. Stated to be 99.9%.
(2) Pentaerythritol tetrananoate. Synthesized from pentaerythritol and nonanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%.

Estimated Error:
Uncertanties in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

Components:

(1) 1,1,1,2-Tetrafluoroethane or HFC-134a; $C_2H_2F_4$; [811-97-2]
(2) 2-Methyl-2,4-pentanediol or hexylene glycol or HEXG; $C_6H_{14}O_2$; [107-41-5]

Original Measurements:

S. I. Tsergounis and M. J. Riley, AIChE Journal **40**, 726–737 (1994) and supplementary material with Microfiche Publication, P. O. Box 3513, NY, NY 10163.

Variables:

T/K = 273.2–353.2
P/kPa = 100–1000

Prepared By:

H. L. Clever

Experimental Values

t/°C	T/K	Pressure (p_1/kPa)	Mol Fraction x_1	Activity a_1	Activity Coefficient $\ln(\gamma_1)$
−5	268.2	238	0.728	0.992	0.309
0	273.2	91	0.095	0.330	1.247
		167	0.195	0.595	1.115
		205	0.296	0.724	0.895
		250	0.441	0.873	0.683
		260	0.460	0.905	0.676
		276	0.527	0.957	0.597
		283	0.639	0.985	0.433
		283	0.724	0.985	0.307
		287	0.916	0.993	0.080
10	283.2	113	0.082	0.295	1.273
		202	0.171	0.516	1.105
		270	0.273	0.679	0.910
		341	0.419	0.844	0.699
		349	0.430	0.862	0.696
		371	0.484	0.911	0.633
		392	0.614	0.958	0.444
		397	0.715	0.969	0.304
		406	0.917	0.989	0.076
20	293.2	137	0.070	0.264	1.329
		239	0.146	0.452	1.126
		338	0.247	0.625	0.927
		453	0.392	0.817	0.736
		356	0.388	0.822	0.750
		480	0.422	0.861	0.712
		523	0.582	0.929	0.468
		539	0.702	0.954	0.308
		550	0.913	0.971	0.062
25	298.2	385	0.246	0.612	0.910
		395	0.255	0.631	0.905
		412	0.273	0.655	0.875
		413	0.271	0.657	0.885
		528	0.412	0.819	0.687
30	303.2	163	0.057	0.240	1.427
		277	0.121	0.398	1.192
		413	0.219	0.578	0.969
30	303.2	416	0.231	0.581	0.922
		432	0.234	0.602	0.943
		446	0.256	0.620	0.884
		448	0.254	0.622	0.896
		557	0.347	0.757	0.781
		568	0.360	0.770	0.760
		586	0.354	0.791	0.805
		587	0.392	0.793	0.705
		680	0.534	0.901	0.523
		740	0.909	0.968	0.063
40	313.2	309	0.101	0.347	1.239
		480	0.200	0.523	0.960
		481	0.193	0.524	0.999
		496	0.197	0.539	1.004
		517	0.220	0.559	0.931
		518	0.218	0.560	0.943
		658	0.300	0.693	0.837
		677	0.289	0.710	0.898
		689	0.325	0.721	0.796
		701	0.346	0.732	0.751
		844	0.473	0.858	0.596
		921	0.656	0.922	0.340
		965	0.902	0.958	0.060
50	323.2	340	0.082	0.306	1.312
		540	0.171	0.470	1.012
		551	0.166	0.479	1.057
		554	0.165	0.481	1.068
		581	0.186	0.502	0.992
		584	0.182	0.505	1.020
		750	0.258	0.629	0.891
		754	0.231	0.632	1.006
		809	0.289	0.672	0.842
		816	0.296	0.677	0.828
60	333.2	368	0.068	0.272	1.392
		593	0.146	0.423	1.061
		602	0.142	0.429	1.106
		607	0.148	0.432	1.075
		639	0.158	0.453	1.055
		639	0.155	0.453	1.070
		816	0.190	0.562	1.086
		830	0.221	0.570	0.946
70	343.2	389	0.059	0.242	1.419
		845	0.189	0.491	0.957
80	353.2	684	0.108	0.353	1.179
		688	0.103	0.355	1.238
		734	0.116	0.376	1.173
		735	0.116	0.376	1.174
		960	0.170	0.475	1.030

Auxiliary Information

Method/Apparatus/Procedure:

The solubility vessel was a thick walled Pyrex tube of known volume sandwiched between two steel plates. It could withstand continuous variations in pressure (100–1800 kPa) and temperature (0–80 °C) without breakage. The vessel assembly was weighed, charged with glycol compound, weighed again, charged with HFC-134a, weighed a third time. The solubility of HFC-134a was measured as mass fraction in the liquid phase and it was converted to mole fraction. The solubility was calculated making the assumptions:
1. The vapor phase was pure HFC-134a.
2. The HFC-134a obeyed a Redlich-Kwong cubic type equation of state.
The experimental procedure was tested by measuring the solubility of chlorodifluoromethane (CFC-22) in tetraethylene glycol dimethyl ether (TGDE). Results agreed within 2% of literature values.

Source and Purity of Material:

(1) 1,1,1,2-Tetrafluoroethane. DuPont Co.
(2) Hexylene glycol. Union Carbide.
No other information specified about components.

Estimated Error:

δT/K = ±0.5
$\delta p/p$ = ±0.2
$\delta m/g$ ±0.01 for both glycol and HFC-134a.
Solubility vessel volume. Two methods agreed within 5%.

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC-134a; $C_2H_2F_4$; [811-97-2]
(2) Triethylene glycol or TRIG; $C_6H_{14}O_4$; [112-27-6]

Original Measurements:
S. I. Tsergounis and M. J. Riley, AIChE Journal **40**, 726–737 (1994) and supplementary material with Microfiche Publications, P. O. Box 3513, NY, NY 10163.

Variables:
T/K = 283.2–353.2
P/kPa = 209–1765

Prepared By:
H. L. Clever

Experimental Values

The solubility of 1,1,1,2-tetrafluoroethane in triethylene glycol

t/°C	T/K	Pressure (p_t/kPa)	Mol Fraction x_1	Activity a_1	Activity Coefficient $\ln(\gamma_1)$
10	283.2	209	0.161	0.534	1.202
		362	0.286	0.891	1.136
		380	0.415	0.931	0.808
		396	0.361	0.968	0.987
20	293.2	258	0.131	0.485	1.308
		312	0.155	0.580	1.317
		421	0.263	0.764	1.067
		514	0.314	0.916	1.071
		536	0.362	0.950	0.966
25	298.2	480	0.229	0.749	1.184
		481	0.230	0.750	1.180
30	303.2	304	0.108	0.434	1.392
		365	0.127	0.516	1.400
		513	0.219	0.703	1.166
		521	0.205	0.713	1.246
		521	0.206	0.713	1.240
		635	0.265	0.849	1.163
		680	0.313	0.901	1.058
40	313.2	341	0.090	0.381	1.441
		588	0.186	0.628	1.219
		589	0.166	0.629	1.332
		592	0.163	0.631	1.353
		733	0.223	0.761	1.228
		811	0.252	0.829	1.192
		905	0.323	0.909	1.034
50	323.2	376	0.073	0.336	1.524
		452	0.086	0.399	1.536
		652	0.131	0.557	1.446
		654	0.130	0.558	1.458
		658	0.155	0.561	1.284
		828	0.182	0.685	1.328
		921	0.204	0.750	1.303
		1054	0.264	0.837	1.154
		1218	0.416	0.939	0.814
60	333.2	403	0.063	0.296	1.541
		705	0.104	0.494	1.559
		708	0.107	0.496	1.537
		714	0.134	0.500	1.317
		906	0.149	0.615	1.419
		1023	0.159	0.649	1.404
		1174	0.216	0.761	1.257
		1424	0.347	0.884	0.935
80	353.2	453	0.046	0.241	1.649
		542	0.058	0.285	1.596
		790	0.069	0.401	1.759
		794	0.066	0.403	1.805
		820	0.096	0.415	1.467
		1037	0.107	0.508	1.560
		1183	0.103	0.567	1.710
		1369	0.150	0.638	1.447
		1765	0.222	0.774	1.250

Auxiliary Information

Method/Apparatus/Procedure:
The solubility vessel was a thick walled Pyrex tube of known volume sandwiched between two steel plates. It could withstand continuous variations in pressure (100–1800 kPa) and temperature (0–80 °C) without breakage. The vessel assembly was weighed, charged with glycol compound, weighed again, charged with HFC-134a, weighed a third time. The solubility of HFC-134a was measured as mass fraction in the liquid phase and it was converted to mole fraction. The solubility was calculated making the assumptions:
1. The vapor phase was pure HFC-134a.
2. The HFC-134a obeyed a Redlich-Kwong cubic type equation of state.
The experimental procedure was tested by measuring the solubility of chlorodifluoromethane (CFC-2) in tetraethylene glycol dimethyl ether (TGDE). Results agreed within 2% of literature values.

Source and Purity of Material:
(1) 1,1,1,2-Tetrafluoroethane. DuPont Co.
(2) Triethylene glycol. Union Carbide.
No other information specified about components.

Estimated Error:
δT/K = ±0.5
$\delta p/p$ = ±0.2
δm/g ± 0.01 for both glycol and HFC-134a.
Solubility vessel volume. Two methods agreed within 5%.

Components:

(1) 1,1,1,2-Tetrafluoroethane or HFC-134a; $C_2H_2F_4$; [811-97-2]
(2) 2,2′-[Oxy*bis*(2,1-ethanediyloxy)]*bis*-ethanol or tetraethylene glycol or TETG; $C_8H_{18}O_5$; [112-60-7]

Original Measurements:

S. I. Tsergounis and M. J. Riley, AIChE Journal **40**, 726–737 (1994) and supplementary material with Microfiche Publications, P. O. Box 3513, NY, NY 10163.

Variables:

T/K = 283.2–353.2
P/kPa = 104–1998

Prepared By:

H. L. Clever

Experimental Values

Solubility of 1,1,1,2-tetrafluoroethane in tetraethylene glycol

t/°C	T/K	Pressure (p_1/kPa)	Mol Fraction x_1	Activity a_1	Activity Coefficient $\ln(\gamma_1)$
10	283.2	104	0.088	0.272	1.132
		238	0.260	0.604	0.842
		265	0.228	0.666	1.074
		296	0.321	0.739	0.834
		316	0.275	0.786	1.050
		343	0.332	0.847	0.937
		357	0.435	0.880	0.704
		395	0.492	0.965	0.674
		396	0.540	0.966	0.583
		410	0.590	0.999	0.535
20	293.2	128	0.068	0.248	1.291
		278	0.215	0.522	0.885
		293	0.214	0.547	0.939
		376	0.241	0.691	1.052
		377	0.279	0.692	0.907
		403	0.305	0.735	0.880
		469	0.392	0.841	0.764
		523	0.452	0.930	0.722
		541	0.501	0.958	0.648
		567	0.557	0.999	0.586
30	303.2	145	0.057	0.213	1.313
		313	0.179	0.446	0.911
		345	0.184	0.489	0.976
		441	0.205	0.614	1.098
		448	0.241	0.6221	0.948
		485	0.262	0.669	1.938
		587	0.341	0.792	0.842
		669	0.397	0.889	0.805
		698	0.452	0.921	0.712
		734	0.517	0.962	0.621
		747	0.575	0.976	0.530
40	313.2	340	0.154	0.380	0.905
		394	0.155	0.436	1.032
		498	0.173	0.540	1.138
		514	0.205	0.556	1.000
		562	0.222	0.602	1.001
		682	0.299	0.715	0.872
		777	0.355	0.800	0.813
		844	0.398	0.858	0.767
		929	0.458	0.929	0.708
		948	0.527	0.945	0.584
50	323.2	363	0.135	0.325	0.877
		434	0.134	0.384	1.056
		547	0.149	0.475	1.162
		572	0.176	0.495	1.033
		628	0.187	0.538	1.056
		768	0.260	0.642	0.903
		897	0.302	0.733	0.888
		986	0.341	0.796	0.843
		1096	0.398	0.864	0.774
		1155	0.466	0.901	0.659
		1233	0.485	0.948	0.670
		1279	0.570	0.974	0.537
60	333.2	383	0.122	0.283	0.840
		469	0.117	0.342	1.072
		590	0.129	0.421	1.186
		624	0.150	0.444	1.082
		685	0.160	0.482	1.102
		850	0.223	0.582	0.959
		997	0.259	0.666	0.945
		1104	0.292	0.724	0.908
		1235	0.345	0.792	0.830
		1354	0.395	0.851	0.768
		1443	0.412	0.893	0.773
		1552	0.495	0.942	0.643
80	353.2	418	0.105	0.224	0.759
		533	0.089	0.281	1.145
		661	0.103	0.342	1.198
		702	0.119	0.361	1.113
		768	0.132	0.391	1.086
		984	0.170	0.486	1.051
		1159	0.197	0.557	1.041
		1292	0.222	0.609	1.011
		1474	0.256	0.676	0.971
		1621	0.305	0.727	0.869
		1765	0.288	0.775	0.991
		1998	0.332	0.844	0.937

Auxiliary Information

Method/Apparatus/Procedure:

The solubility vessel was a thick walled Pyrex tube of known volume sandwiched between two steel plates. It could withstand continuous variations in pressure (100–1800 kPa) and temperature (0–80 °C) without breakage. The vessel assembly was weighed, charged with glycol compound, weighed again, charged with HFC-134a, weighed a third time. The solubility of HFC-134a was measured as mass fraction in the liquid phase and it was converted to mole fraction. The solubility was calculated making the assumptions:
1. The vapor phase was pure HFC-134a.
2. The HFC-134a obeyed a Redlich-Kwong cubic type equation of state.
The experimental procedure was tested by measuring the solubility of chlorodifluoromethane (CFC-22) in tetraethylene glycol dimethyl ether (TGDE). Results agreed within 2% of literature values.

Source and Purity of Material:

(1) 1,1,1,2-Tetrafluoroethane. DuPont Co.
(2) Tetraethylene glycol. Aldrich Chemicals.
No other information specified about components.

Estimated Error:

δT/K = ±0.5
$\delta p/p$ = ±0.2
δm/g ± 0.01 for both glycol and HFC-134a.
Solubility vessel volume. Two methods agreed within 5%.

Components:

(1) 1,1,1,2-Tetrafluoroethane or HFC-134a; $C_2H_2F_4$; [811-97-2]
(2) Tetraethylene glycol dimethyl ether or TGDE; $C_{10}H_{22}O_5$; [143-24-8]

Original Measurements:

S. I. Tsergounis and M. J. Riley, AIChE Journal **40**, 726–737 (1994) and supplementary material with Microfiche Publications, P. O. Box 3513, NY, NY 10163.

Variables:

T/K = 273.2–353.2
P/kPa = 74–1693

Prepared By:

H. L. Clever

Experimental Values

t/°C	T/K	Pressure (p_t/kPa)	Mol Fraction x_1	Activity a_1	Activity Coefficient $\ln(\gamma_1)$
0	273.2	144	0.662	0.516	−0.249
10	283.2	74	0.316	0.194	−0.487
		93	0.360	0.317	−0.389
		102	0.426	0.267	−0.469
		119	0.437	0.309	−0.348
		122	0.469	0.244	−0.389
		153	0.537	0.395	−0.306
		194	0.626	0.496	−0.233
		212	0.663	0.540	−0.206
		214	0.652	0.542	−0.184
		254	0.703	0.641	−0.094
		267	0.749	0.672	−0.109
		305	0.800	0.760	−0.052
20	293.2	103	0.301	0.200	−0.408
		128	0.343	0.248	−0.323
		142	0.410	0.274	−0.405
		156	0.408	0.301	−0.304
		175	0.450	0.335	−0.295
		220	0.519	0.417	−0.218
		274	0.611	0.514	−0.172
		294	0.652	0.549	−0.172
		294	0.640	0.549	−0.153
		347	0.694	0.640	−0.081
		368	0.741	0.676	−0.092
		418	0.795	0.6760	−0.044
30	303.2	136	0.282	0.202	−0.334
		174	0.321	0.255	−0.230
		192	0.389	0.281	−0.325
		201	0.370	0.294	−0.230
		227	0.432	0.331	−0.268
		295	0.498	0.422	−0.165
		374	0.593	0.527	−0.119
		391	0.625	0.549	−0.128
		391	0.638	0.551	−0.147
		471	0.679	0.652	−0.041
		490	0.732	0.675	−0.081
		569	0.788	0.772	−0.020
40	313.2	169	0.265	0.195	−0.308
		221	0.296	0.252	−0.163
		243	0.368	0.277	−0.286
		243	0.332	0.277	−0.183
		294	0.408	0.331	−0.208
		378	0.473	0.420	−0.120
		484	0.572	0.526	−0.083
		506	0.604	0.548	−0.097
		509	0.620	0.551	−0.117
		608	0.663	0.646	−0.025
		635	0.719	0.666	−0.077
		744	0.778	0.771	−0.009
50	323.2	207	0.244	0.192	−0.242
		270	0.271	0.246	−0.097
		283	0.293	0.258	−0.130
		298	0.332	0.270	−0.207
		363	0.382	0.326	−0.159
		467	0.446	0.412	−0.080
		599	0.546	0.516	−0.057
		628	0.582	0.538	−0.079
		643	0.597	0.550	−0.083
		761	0.641	0.637	−0.005
		817	0.702	0.678	−0.034
		954	0.765	0.772	−0.009
60	333.2	246	0.222	0.186	−0.181
		318	0.246	0.237	−0.035
		320	0.271	0.238	−0.129
		353	0.321	0.262	−0.201
		428	0.357	0.314	−0.129
		525	0.430	0.379	−0.126
		722	0.519	0.505	−0.028
		764	0.557	0.530	−0.049
		789	0.570	0.545	−0.044
		931	0.614	0.628	+0.023
		1016	0.678	0.676	−0.002
		1188	0.748	0.768	+0.026
80	353.2	314	0.186	0.171	−0.086
		383	0.200	0.206	+0.031
		411	0.197	0.220	+0.113
		462	0.273	0.246	−0.104
		552	0.309	0.290	−0.062
		746	0.348	0.381	+0.090
		983	0.448	0.485	0.081
		1027	0.495	0.504	0.018
		1077	0.509	0.525	0.031
		1279	0.549	0.604	0.096
		1436	0.622	0.663	0.064
		1693	0.702	0.750	0.066

Auxiliary Information

Method/Apparatus/Procedure:

The solubility vessel was a thick walled Pyrex tube of known volume sandwiched between two steel plates. It could withstand continuous variations in pressure (100–1800 kPa) and temperature (0–80 °C) without breakage. The vessel assembly was weighed, charged with glycol compound, weighed again, charged with HFC-134a, weighed a third time. The solubility of HFC-134a was measured as mass fraction in the liquid phase and it was converted to mole fraction. The solubility was calculated making the assumptions:
1. The vapor phase was pure HFC-134a.
2. The HFC-134a obeyed a Redlich-Kwong cubic type equation of state.
The experimental procedure was tested by measuring the solubility of chlorodifluoromethane (CFC-22) in tetraethylene glycol dimethyl ether (TGDE). Results agreed within 2% of literature values.

Source and Purity of Material:

(1) 1,1,1,2-Tetrafluoroethane. DuPont Co.
(2) Tetraethylene glycol dimethyl ether. Aldrich Chemicals.
No other information specified about components.

Estimated Error:

δT/K = ±0.5
$\delta p/p$ = ±0.2
δm/g ± 0.01 for both glycol and HFC-134a.
Solubility vessel volume. Two methods agreed within 5%.

Components:

(1) 1,1,1,2-Tetrafluoroethane or HFC-134a; $C_2H_2F_4$; [811-97-2]
(2) Polyalkylene-glycol oil or PAG; RO-$(CH_2C(CH_3)HO)_5$-H

Original Measurements:

T. Sato, Y. Takaishi, and K. Oguchi, Trans. JSRAE **18**(3), 273–278 (2001).

Variables:

T/K = 283.15–333.15
P_1 /kPa = 0.0999–1.6787

Prepared By:

H. L. Clever

Experimental Values

Temperature (T/K)	Partial Pressure (p_1 /MPa)	Weight Fraction w_1	Temperature (T/K)	Partial Pressure (p_1 /MPa)	Weight Fraction w_1
283.15	0.4126	1.000	303.15	0.7672	1.000
	0.4091	0.949		0.7654	0.949
	0.4080	0.898		0.7619	0.897
	0.4059	0.848		0.7602	0.846
	0.4079	0.796		0.7588	0.794
	0.4046	0.746		0.7557	0.743
	0.4039	0.696		0.7525	0.692
	0.3987	0.638		0.7424	0.627
	0.3940	0.586		0.7329	0.574
	0.3846	0.535		0.7145	0.522
	0.3700	0.484		0.6905	0.470
	0.3539	0.433		0.6539	0.420
	0.3330	0.383		0.6132	0.369
	0.3039	0.334		0.5635	0.320
	0.2759	0.284		0.5051	0.272
	0.2354	0.236		0.4365	0.225
	0.1916	0.188		0.3575	0.178
	0.0999	0.093		0.1872	0.088
293.15	0.5697	1.000	313.15	1.0146	1.000
	0.5678	0.949		1.0117	0.948
	0.5653	0.898		1.0076	0.896
	0.5636	0.847		1.0055	0.845
	0.5633	0.795		1.0038	0.792
	0.5604	0.745		1.0002	0.741
	0.5581	0.694		0.9963	0.690
	0.5511	0.633		0.9820	0.619
	0.5446	0.581		0.9685	0.565
	0.5314	0.529		0.9419	0.512
	0.5139	0.478		0.9071	0.460
	0.4884	0.427		0.8557	0.410
	0.4590	0.377		0.7994	0.360
	0.4223	0.328		0.7319	0.311
	0.3800	0.279		0.6537	0.264
	0.3279	0.231		0.5637	0.218
	0.2683	0.183		0.4612	0.173
	0.1402	0.091		0.2430	0.085
323.15	1.3149	1.000	333.15	1.6787	1.000
	1.3106	0.948		1.6725	0.947
	1.3059	0.896		1.6678	0.894
	1.3035	0.843		1.6657	0.841
	1.3019	0.790		1.6649	0.787
	1.2983	0.739		1.6614	0.736
	1.2938	0.687		1.6567	0.683
	1.2721	0.609		1.6207	0.594
	1.2517	0.554		1.5884	0.538
	1.2124	0.500		1.5281	0.485
	1.1619	0.448		1.4532	0.434
	1.0895	0.398		1.3526	0.385
	1.0126	0.349		1.2498	0.337
	0.9221	0.301		1.1314	0.290
	0.8202	0.255		1.0023	0.246
	0.7043	0.210		0.8570	0.202
	0.5750	0.167		0.6980	0.160
	0.3020	0.082		0.3676	0.078

Auxiliary Information

Method/Apparatus/Procedure:

The experimental apparatus consists of a glass equilibrium cell of a volume of 17.93 cm^3, a temperature measuring system and a pressure measuring system. The system is completely miscible over the range of temperature and pressure studied here. The authors compare the present results on HFC-134a in the polyalkylene-glycol oil with HFC-134a in polyol ester oil[1] and naphthenic oil[2] in Fig. 3 of the paper. The first two systems show only small differences while the naphthenic oil shows liquid-liquid immiscibility at 323.15 K at about 0.1 weight fraction HCF-134a. Figure 3 uses mole fraction, but we did not find a mole weight for the PAG used in this study.

Source and Purity of Material:

(1) HFC-134a. Purity stated to be 99.9 wt %.
(2) Polyalkylene-glycol-oil. Density at 288.15 K is 982 kg m^{-3}; Kinematic viscosity is:
313.15 K 33.54 mm^2 s^{-1} and
373.15 K 6.942 mm^2 s^{-1}.

Estimated Error:

δT/K = ±0.015
δp_1/kPa = ±8
δw_1 /w_1 = ±0.01

References:

[1]Y. Takaishi, H. Nakagawa, and K. Oguchi, Trans. JAR **10**(1), 67–73 (1993).
[2]Y. Tanaka, H. Kawachi, C. Takata, H. Kabota, and T. Makita, Proc. 2nd Asian Thermophysical Properties Conference, Sapporo, 1989, pp. 375–379.

Components:
(1) 1,1,1,2-Tetrafluoroethane or 134a; $C_2H_2F_4$; [811-97-2]
(2) Polyolester based oil; $C(CH_2OOCR)_4$ with $R=(C_5-C_{10})$; Mol wt ~610.

Original Measurements:
Y. Takaishi, H. Nakagawa, and K. Oguchi, Trans. JAR **10**(1), 67–73 (1993).

Variables:
T/K=263.15–323.15
P_1 /MPa=0.0980–1.314

Prepared By:
H. L. Clever

Experimental Values

Temperature (T/K)	Partial Pressure (p_1 /MPa)	Weight Fraction w_1	Mole Fraction x_1
263.15	0.0980*	0.150	0.513
	0.136	0.233	0.645
	0.163	0.311	0.730
	0.182	0.399	0.799
	0.194	0.505	0.859
	0.198	0.615	0.905
	0.198	0.698	0.933
	0.199	0.832	0.967
	0.200	0.899	0.982
	0.202	1.000	1.000
283.15	0.196	0.147	0.506
	0.271	0.229	0.639
	0.326	0.306	0.725
	0.368	0.395	0.796
	0.392	0.501	0.857
	0.402	0.612	0.904
	0.405	0.695	0.932
	0.407	0.831	0.967
	0.411	0.899	0.982
	0.415	1.000	1.000
303.15	0.341	0.142	0.497
	0.482	0.222	0.631
	0.584	0.299	0.718
	0.663	0.388	0.791
	0.715	0.494	0.854
	0.739	0.606	0.902
	0.745	0.691	0.930
	0.751	0.829	0.967
	0.753	0.897	0.981
	0.769	1.000	1.000
323.15	0.521	0.137	0.487
	0.758	0.214	0.620
	0.929	0.289	0.708
	1.078	0.377	0.783
	1.196	0.483	0.848
	1.251	0.598	0.899
	1.265	0.683	0.928
	1.279	0.825	0.966
	1.292	0.895	0.981
	1.314	1.000	1.000

*Pressure measured with a mercury manometer.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consists of a glass equilibrium cell of 17.93 cm^3 volume, and a temperature- and a pressure-measuring system. The system shows no liquid-liquid immiscibility under the conditions studied. A correlation equiation is given for the pressure, wt fraction and temperature. The thre dimensional p, wt fraction and T is depicted in Fig. 7 of the paper.

Source and Purity of Materials:
(1) HFC-134a. Purity stated to be 99.9 wt %.
(2) Polyolester based oil. Mol wt 610; Density 973.5 kg m^{-3} at 288.15 K; Kinematic viscosity 31 mm^2 s^{-1} at 313.15 K.

Estimated Error:
δT/K=±0.010
δp_1 /kPa=±5
δw_1 /w_1=±0.005

References:
Note: Trans. JAR is Trans. Japn. Assoc. Refrig. Eng. Or see Nippon Reito Kucho Gakki Ronbunshu.

Components:

(1) Difluoromethane or R-32; CH_2F2; [75-10-5]; (30 mass %) +1,1,1,2-Tetrafluoroethane or R-134a; $C_2H_2F_4$; [811-97-2]; (70 mass %).
(2) Polyol ester mixture; $C(CH_2OOCR)_4$ with R of $n=5-10$; Mole wt 610

Original Measurements:

Y. Takaishi and K. Oguchi, Proceedings-International Congress of Refrigeration, 20th, IIR/HF, Sydney, 1999, Vol. II, paper 402.

Variables:

T/K=263.15–323.15
p_1 /MPa=0.392–2.126

Prepared By:

H. L. Clever

Experimental Values

The R-32/R-134a (30/70 mass %)+Polyol ester oil system

Temperature (T/K)	Partial Pressure (p_1 /MPa)	Weight Fraction w_1	Temperature (T/K)	Partial pressure (p_1 /MPa)	Weight Fraction w_1
263.15	0.392	1.000	303.15	1.300	1.000
	0.389	0.903		1.285	0.901
	0.389	0.797		1.270	0.794
	0.371	0.587		1.210	0.581
	0.353	0.334		1.095	0.327
	0.315	0.250		0.964	0.245
	0.222	0.146		0.641	0.142
283.15	0.742	1.000	323.15	2.126	1.000
	0.734	0.902		2.097	0.901
	0.727	0.796		2.063	0.791
	0.696	0.585		1.965	0.575
	0.651	0.331		1.721	0.325
	0.575	0.247		1.491	0.239
	0.396	0.144		0.970	0.139

Auxiliary Information

Method/Apparatus/Procedure:

The experimental apparatus consists of a glass equilibrium cell of inner volume 17.93 cm^3 and temperature- and presure-measuring systems. The apparatus is used to measure vapor presssure of pure liquids, solubility of refrigerant+oil mixtures and liquid-liquid phase separations if they ocur. The apparatus is described in detail in an earlier paper.[1] The solution sample is prepared by weight. The oil is added and weighed, the cell is evacuated, the refrigerant mixture is prepared in a steel cylinder and transferred to the cell. The cell is filled so that 90% of the volume is ocupied by liquid. Thus the concentration in the liquid phase can be the same as that initially charged into the cell. No liquid-liquid immiscibility is observed under the conditions of the study. A correlation equation is given.

Source and Purity of Material:

DuPont-Mitui Fluorochemicals Co., Ltd., Tokyo, Japan provided the R-32 and R-134a.
(1) Difluoromethane or R-32. Purity stated to be 99.99 mass %; 1,1,12-Tetrafluoroethane or R-134a. Purity stated to be 99.9 mass %.
(2) Polyol ester lubricating oil. JOMO Technical Research Center Co., Ltd. Saitama, Japan. Mol. wt. 610; Density is 974 kg m^{-3} at 298.15 K; Kinematic viscosity is 31 mm^2 s^{-1} at 313.15 K and 5 mm^2 s^{-1} at 373.15 K.

Estimated Error:

δT/K=±0.010
δp_1 /kPa=±5
$\delta w_1/w_1$=±0.04 or less.

References:

[1]Y. Takaishi, H. Nakagawa, and K. Oguchi, Trans. JAR **10**(**1**), 67–73 (1993).

Components:

(1) Difluoromethane or R-32; CH_2F_2; [75-10-5]; (23 mass %) +Pentafluoroethane or R-125a; C_2HF_5; ; (25 mass %); C_2HF_5; [354-33-6]; (25 mass %); +1,1,1,2-Tetrafluoroethane or R-134a; $C_2H_2F_4$; [811-97-2]; (52 mass %).
(2) Polyol ester mixture; $C(CH_2OOCR)_4$ with R of $n=5-10$; Mole wt 610.

Original Measurements:

Y. Takaishi and K. Oguchi, Proceedings-International Congress of Refrigeration, 20th, IIR/HF, Sydney, 1999, Vol. II, paper 402.

Variables:

T/K=263.15–323.15
p_1 /MPa=0.431–1.727

Prepared By:

H. L. Clever

Experimental Values

The R-32/R-125a/R-134a (23/25/52 mass %)+Polyol ester oil system

Temperature (T/K)	Partial Pressure (p_1 /MPa)	Weight Fraction w_1	Temperature (T/K)	Partial Pressure (p_1 /MPa)	Weight Fraction w_1
263.15	0.431	1.000	293.15	1.041	1.000
	0.410	0.737		1.013	0.732
	0.368	0.509		0.920	0.499
	0.282	0.240		0.668	0.224
273.15	0.590	1.000	303.15	1.350	1.000
	0.565	0.736		1.333	0.729
	0.511	0.506		1.199	0.494
	0.380	0.235		0.849	0.216
283.15	0.791	1.000	323.15	1.727	1.000
	0.767	0.734		1.711	0.725
	0.697	0.504		1.536	0.488
	0.515	0.230		1.059	0.207

Auxiliary Information

Method/Apparatus/Procedure:

The experimental apparatus consists of a glass equilibrium cell of inner volume 17.93 cm^3 and temperature- and presure-measuring systems. The apparatus is used to measure vapor presssure of pure liquids, solubility of refrigerant+oil mixtures and liquid-liquid phase separations if they ocur. The apparatus is described in detail in an earlier paper.[1] The solution sample is prepared by weight. The oil is added and weighed, the cell is evacuated, the refrigerant mixture is prepared in a steel cylinder and transferred to the cell. The cell is filled so that 90% of the volume is occupied by liquid. Thus the concentration in the liquid phase can be the same as that initially charged into the cell. No liquid-liquid immiscibility is observed under the conditions of the study. The results are correlated in an equation that is a function of temperature, weight fraction, and pressure.

Source and Purity of Material:

DuPont-Mitui Fluorochemicals Co., Ltd., Tokyo, Japan provided the R-32, R-125, and R-134a.
(1) Difluoromethane or R-32. Purity stated to be 99.99 mass %; Pentafluoroethane or R-125, Purity stated to be 99.86; 1,1,12-Tetrafluoroethane or R-134a. Purity stated to be 99.99 mass %.
(2) Polyol ester lubricating oil. JOMO Technical Research Center Co., Ltd. Saitama, Japan. Mol. wt. 610; Density is 974 kg m^{-3} at 298.15 K; Kinematic viscosity is 31 mm^2 s^{-1} at 313.15 K and 5 mm^2 s^{-1} at 373.15 K.

Estimated Error:

δT/K=±0.010
δp_1 /kPa=±5
$\delta w_1/w_1$=±0.04 or less.

References:

[1]Y. Takaishi, H. Nakagawa, and K. Oguchi, Trans. JAR **10**(1), 67–73 (1993).

Components:
(1) 1,1,1,2-Tetrafluoroethane or HFC-134a; $C_2H_2F_4$; [811-97-2]
(2) Various commercial lubricants

Original Measurements:
Y. Yamamoto, S. Gondo, and J. Kim, Tribology Trans. **44**, 209–214 (2001).

Variables:
T/K=293–298
P_1 /kPa=98 (gage)

Prepared By:
H. L. Clever

Experimental Values

The solubility of 1,1,1,2-tetrafluoroethane was measured in nine lubricating oils. They were classed as follows:

Mineral oils MO32 and MO68,

Polyalkylenes PAG32 and PAG68,

Linear polyolestors L-POE32 and L-POE68 and branched polyolestor HS-POE68, and
Polyvinyl ethers PVE32 and PVE68.

The results were in a bar graph, which was read to the nearest 0.1 mass % by the compiler.

Lubricating Oil	Solubility (Mass %)
MO32	1.2
MO68	1.1
PAG32	4.2
PAG68	3.7
L-POE32	4.3
L-POE68	2.8
HS-POE68	4.6
PVE32	4.9
PVE68	4.8

Some properties of the lubricating oils.

Property/Oil	MO32	MO68	PAG32	PAG68	L-POE32	L-POE68	HS-POE68	PVE32	PVE68
Viscosity At 40 °C, cSt	36.95	67.6	28.98	70.78	24.52	65.94	70.17	30.70	63.46
Viscosity At 100 °C, cSt	5.64	9.06	5.92	11.62	5.07	12.31	8.48	4.91	7.62
Viscosity Index	87	105	155	159	139	188	89	67	77
Density At 15 °C, g cm^{-3}	0.868	0.868	0.959	0.966	0.993	0.927	0.960	0.904	0.925
Mean Molecular Weight	460	498	900	1300	650	730	750	610	830

Auxiliary Information

Method/Apparatus/Procedure:
The oils were degassed by pumping with a rotary vacuum pump for 30 min. They were saturated by blowing through the solute gas at a gage pressure of 98 kPa. A blowing time of 10 min at 100 cm^3 min^{-1} insured saturation. The weight increase was measured. The temperature increased from the initial 20 °C because of the exothermic solution process.

Source and Purity of Material:
(1) HFC-134a. Nothing specified.
(2) Lubricating oils. Idemitsu Kosan Co. Properties given above, in addition the cohesive energy density (graph), viscosity reduction on dissolving gas and change in lubricant film thickness with dissolved gas is given in paper.

Estimated Error:
Nothing specified.

Components:
(1) 1,1,1,2-Tetrafluoroethane or R-134a, $C_2H_2F_4$; [811-97-2]
(2) Various lubricating oils.

Original Measurements:
Miscellaneous References.
See below.

Variables:

Prepared By:
H. L. Clever

Experimental Values

The following papers give solubility data in graph form only. Data sheets were not prepared, but the data seemed useful enough to note the references here.

[1]R. H. P. Thomas, H. T. Pham, and W.-T. Wu, "Solubility and viscosity of R-134a refrigerant/lubricating mixtures;" ASHRAE J. 37–38 (1991).

[2]R. H. P. Thomas and H. T. Pham, "On environmentally safer refrigerant/lubricant mixtures," ASHRAE Trans. **97**, 783–788 (1992).

[3]K. Inoue and A. Iwamoto, "Mutual solubility of HFC-134a and synthetic ester base stocks," Sekiyu Gakkaishi **35**(1), 76–83 (1992); Chem. Abstr. **116**, 132451.

The solubility of tetraesters of pentaerythriotol in HFC-134a was studied by analysis of the three dimensional solubility parameters and ^{1}H-NMR spectra. The liquid system shows both upper and lower phase separation temperature.

[4]T. Hitano, Y. Maruiwa, and T. Hamada, "Solubility behavior of HFC-134a and PAG oil," Reito **67**(12), 1360–1366 (1992); Chem. Abstr. **118**, 257760.

Studies of liquid and liquid-liquid phases.

[5]V. Z. Geller and K. E. Davis, "Solubility and viscosity of refrigerant/POE lubricant mixtures," Proceedings-International Congress of Refrigeration, 19th, The Hague, Aug 20–25, 1995, Vol. 4A, pp. 568–574; Chem. Abstr. **127**, 192378.

Present graphical data on R22, R32, R134a, R404a, R407c, R410, and R507 from −20 °C to 120 °C and pressures up to 5 MPa.

[6]R. H. P. Thomas, W. T. Wu, and H. T. Pham, "The solubility of R134a with modified polyglycols," Actes Congr. Int. Froid, 18th, 1991, Vol. 2, pp. 412–415; Chem. Abstr. **120**, 227676.

Solubility of R134a in modified polyglycol BRL-150 from 10 °C to 70 °C and pressures up to 2000 kPa.

3.12. 1,1,2,2-Tetrafluorethane

Components:
(1) 1,1,2,2-Tetrafluoroethane or HFC-134b; $C_2H_2F_4$; [359-35-3]
(2) Tetraethylene glycol dimethyl ether; $C_{10}H_{22}O_5$; [143-24-8]

Original Measurements:
S. V. R. Mastrangelo, ASHRAE J. **1**(10), 64–68 (1960).

Variables:
T/K = 301.4–359.6
p_1 /MPa = 0.0290–0.506

Prepared By:
H. L. Clever

Experimental Values

t/°C	T/K	Pressure (p_1 /psia)	Vapor Pressure (P_1°/psia)	Mole Fraction x_1	Activity $a_1 = p_1/p_1$°	Activity Coefficient
28.8	302.0	4.206	86.29	0.1875	0.04874	0.2599
28.2	301.4	7.710	84.72	0.2942	0.09101	0.3093
28.6	301.8	10.98	85.77	0.3624	0.1280	0.3532
28.2	301.4	13.40	84.72	0.4102	0.1582	0.3857
28.6	301.8	15.66	85.77	0.4422	0.1826	0.4111
28.6	301.8	17.22	85.77	0.4647	0.2008	0.4321
28.6	301.8	27.69	85.77	0.5622	0.3228	0.5701
28.7	301.9	32.2	86.03	0.6235	0.3743	0.6003
28.2	301.4	40.1	84.72	0.6758	0.4733	0.7004
28.6	301.8	48.1	85.77	0.7398	0.5608	0.7580
56.7	329.9	15.22	187.7	0.2260	0.08109	0.3588
56.3	329.5	22.26	185.8	0.3000	0.1198	0.3951
56.0	329.2	31.2	184.4	0.3824	0.1692	0.4425
56.0	329.2	45.0	184.4	0.4769	0.2440	0.5116
56.0	329.2	61.6	184.4	0.5653	0.3341	0.5910
56.0	329.2	67.3	184.4	0.5906	0.3650	0.6180
86.4	359.6	19.08	348	0.1305	0.05483	0.4202
86.2	359.4	31.6	348	0.2076	0.09080	0.4374
86.3	359.5	49.9	348	0.2984	0.1434	0.4806
86.2	359.4	66.2	348	0.3685	0.1902	0.5161
86.2	359.4	73.4	348	0.3941	0.2109	0.5351

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consists of a stainless steel vessel (22.74 cm^3) with several steel balls for agitation and a vessel equipped with a valve, which contains the solute. A portion of the solute gas is transferred to the solvent vessel and closed. The solute in the connecting tubes is condensed back to the solute vessel and weighed. The loss of weight in the solute dissolved. The solvent vessel is agitated until equilibrium is reached and the equilibrium pressure is read on a mercury manometer or a pressure gage. Many more details in the paper.

Source and Purity of Material:
(1) 1,1,2,2-Tetrafluoroethane. The middle cuts in precise distillations. IR, mas spectrometry, and GLC used to determine impurities. Purity stated to be 99.5% or better.
(2) Tetraethylene glycol dimethyl ether. Ansul ether E-181. Used as received.

Estimated Error:
δT/K = ±0.1
δp_1 /psi = ±0.2 above 15 psig; below 15 psig mercury manometer used.

3.13. 1,1,1-Tifluoroethane

Components:
(1) 1,1,1-Trifluoroethane or HFC143a; $C_2H_3F_3$; [420-46-2]
(2) Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 293.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution γ^∞
293.15	4.12	4.81
303.15	4.72	4.46
323.15	6.00	4.00
343.15	7.30	3.89
363.15	8.60	–

Henry's constant He/MPa = $\lim_{x_1 \to 0} (f_1$ /MPa$)/x_1$

Isochoric Method. At equilibrium $f_1{}^l = f_1{}^v = \varphi_1{}^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1{}^\infty = (He_{1,2})/f^{*l}{}_1$. Not derived for temperatures of the solute when it is above its critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Material:
(1) 1,1,1-Trifluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Hexadecane. Lancaster Synthesis. Stated to be of 99% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = \pm 0.02$ at low pressure;
$= \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1-Trifluoroethane or HFC143a; $C_2H_3F_3$ [420-46-2]
(2) 2,6,10,14-Tetramethylepentadecane; $C_{19}H_{40}$; [1921-70-6]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 293.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution
293.15	3.29	3.84
303.15	3.82	3.61
323.15	4.97	3.32
343.15	6.15	3.29
363.15	7.37	–

Henry's constant $He/\text{MPa} = \lim_{x_1 \to 0} (f_1/\text{MPa})/x_1$

Isochoric Method. At equilibrium $f_1^l = f_1^v = \varphi_1^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1^\infty = (He_{1,2})/f^{*l}_1$. Not derived for temperatures of the solute when it is above its critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Material:
(1) 1,1,1-Trifluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) 2,6,10,14-Tetramethylpentadecane. Sigma Chemical Co. St. Louis, MO. Stated to be of 98% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1-Trifluoroethane or HFC143a; $C_2H_3F_3$; [420-46-2]
(2) Eicosane; $C_{20}H_{42}$; [112-95-8]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 323.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution γ^∞
323.15	5.78	3.85
343.15	7.03	3.74
363.15	8.31	–

Henry's constant $He/\text{MPa} = \lim_{x_1 \to 0} (f_1/\text{MPa})/x_1$

Isochoric Method. At equilibrium $f_1^l = f_1^v = \varphi_1^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1^\infty = (He_{1,2})/f^{*l}_1$. Not derived for temperatures of the solute when it is above its critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Material:
(1) 1,1,1-Trifluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Eicosane. Sigma Chemical Co. St. Louis, MO. Stated to be of 99% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1,1-Trifluoroethane or HFC143a; $C_2H_3F_3$; [420-46-2]
(2) Pentaerythritol tetrapentanonate ester; $C_{25}H_{44}O_8$; [15834-04-5] *Chem. Abstr.* name: Pentanoic 2,2-*bis*[(1-oxypentyl)oxylmethyl]-1,3-propanediyl ester.

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823–828 (1999).

Variables:
T/K = 303.15–363.15
p_1 /MPa = 0.05–1.9

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1MPa	Mol Fraction x_1
303.15	0.0877	0.0630	343.16	0.1216	0.0440
303.18	0.1525	0.1059	343.15	0.2119	0.0748
303.16	0.4084	0.2541	343.17	0.5729	0.1808
303.17	0.5525	0.3375	343.17	0.7953	0.2514
303.14	0.6900	0.4058	343.12	1.0133	0.3073
303.13	0.8557	0.4855	343.13	1.2738	0.3716
303.15	1.1403	0.6239	343.17	1.6965	0.4604
323.27	0.1060	0.0526	363.21	0.1352	0.0370
323.28	0.1846	0.0889	363.25	0.2350	0.0636
323.27	0.4988	0.2137	363.24	0.6339	0.1531
323.27	0.6867	0.2903	363.25	0.8838	0.2172
323.25	0.8691	0.3533	363.19	1.1292	0.2664
323.24	1.0906	0.4249	363.18	1.4093	0.3269
323.27	1.4762	0.5377	363.23	1.8427	0.3907

Henry's constant was calculated for the 8 points at pressures below 0.24 MPa and fitted to the equation $\ln(He_{1,2}/\text{MPa}) = \ln(2.332 \pm 0.020) - (1750 \pm 42)[1/(T/\text{K}) - 1/333.15]$. The CH_2F_2 activity coefficients at infinite dilution are: $(T/\text{K})/\gamma^{\infty}$ 303.2/1.29; 323.2/1.30; 343.2/1.39.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from pressure changes in a gas system of known volume, observed during the absorption of the gas. The apparatus consists of three sections. (*i*) A liquid bath thermostat 1 containing the equilibrium cell with a magnetic stirrer; (*ii*) liquid bath thermostat 2 with a gas bottle of calibrated volume; (*iii*) an air bath thermostat with a pressure transmitter and connections between the first two sections and to a gas storage and a vacuum pump. More details of the apparatus, the experimental technique, and the treatment of the data are in an earlier paper of the authors.[1]

Source and Purity of Material:
(1) 1,1,1-Trifluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Pentaerythritol tetrapentanonate ester. Synthesized[2] by a reaction between valeric acid and pentaerythirtol catalyzed with p-toluenesulfonic acid in a p-xylene solvent. The product was vacuum distilled. NMR and IR results gave a purity >95%.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p_1/p_1 = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]K. D. Black and F. D. Gunstone, Chem. Phys. Lipids **56**, 169 (1990).

Components:
(1) 1,1,1-Trifluoroethane or HFC143a; $C_2H_3F_3$ [420-46-2]
(2) Pentaerythitol tetra-2-ethylbutanoate; $C_{29}H_{52}O_8$; [139116-32-8]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 323.15–363.25
p_1 /MPa = 0.1651–1.9669

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1MPa	Mol Fraction x_1
303.15	The		343.26	0.1894	0.0669
	solvent		343.24	0.1955	0.0723
	is a solid		343.29	0.2490	0.0910
	at this		343.29	0.4769	0.1711
	temperature		343.27	0.9292	0.3080
			343.26	1.2634	0.3967
			343.27	1.7884	0.5178
323.09	0.1651	0.0861	363.23	0.2089	0.0577
323.08	0.1707	0.0886	363.22	0.2158	0.0595
323.12	0.2202	0.1119	363.25	0.2713	0.0747
323.12	0.4173	0.2025	363.25	0.5253	0.1452
323.12	0.8163	0.3615	363.26	1.0124	0.2625
323.11	1.0780	0.4527	363.25	1.4050	0.3452
323.11	1.5164	0.5882	263.24	1.9669	0.4499

$\ln(H_{2,1}/\text{MPa}) = (2.231 \pm 0.010) - (1841 \pm 29)[1/(T/\text{K}) - 1/333.15]$.
Solvent Chem. Abstr. Name: 2,2-bis[(2-ethyl-1-oxybutoxy) methyl]-1,3-propanediyl ester of 2ethylbutanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) 1,1,1-Trifluoroethane. DuPont de Nemours, Dodrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetra-2-ethylbutanote. Synthesized from pentaerythriiol and 2-ethyl-butanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%. Melting point 310–312 K.

Estimated Error:
Uncertanties in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure: <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) 1,1,1-Trifluoroethane or HFC143a; $C_2H_3F_3$; [420-46-2]
(2) Pentaerythritol tetra-2-ethylhexanoate; $C_{37}H_{68}O_8$; [7299-99-2]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 303.11–363.25
p_1 /MPa = 0.0751–0.8732

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1MPa	Mol Fraction x_1
303.11	0.0751	0.1576	343.22	0.1242	0.1163
303.13	0.0842	0.1739	343.23	0.1388	0.1294
303.14	0.1007	0.2053	343.25	0.1681	0.1534
303.13	0.2618	0.4544	343.15	0.4371	0.3435
303.13	0.4006	0.5865	343.12	0.7368	0.4817
303.15			343.16		
323.05	0.1000	0.1367	363.22	0.1451	0.0990
323.07	0.1116	0.1516	363.21	0.1626	0.1100
323.08	0.1347	0.1794	363.22	0.1971	0.1307
323.23	0.3552	0.3999	363.24	0.5015	0.2930
323.23	0.5739	0.5388	363.25	0.8732	0.4221
323.27			363.23		

$\ln(H_{2,1}/\text{MPa}) = (2.087 \pm 0.025) - (1616 \pm 60)[1/(T/\text{K}) - 1/333.15]$

Solvent Chem. Abstr. Name: 2,2-bis[(2-ethyl-1-oxyhexyl)oxylmethyl]-1,3-propanediyl ester of 2-ethylhexanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant, and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (>0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Materials:
(1) 1,1,1,2-Tetrafluoroethane. ICI Chemicals and Polymers, Ltd., Runcorn, Cheshire, U.K. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylhexanoate. Synthesized from pentaerythriiol and 2-ethylhexanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >90%. Contains 5%–10% di- and tri-esters.

Estimated Error:
Uncertaines in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure; <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) 1,1,1-Trifluoroethane or HFC143a; $C_2H_3F_3$; [420-46-2]
(2) Pentaerythritol tetrananoate; $C_{41}H_{76}O_8$; [14450-05-6]

Original Measurements:
Å Wahlström and L. Vamling, L. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 303.00–363.33
p_1 /MPa = 0.1353–1.9742

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1/MPa	Mol Fraction x_1
303.16	0.1353	0.1020	343.21	0.1728	0.0718
303.15	0.1741	0.1269	343.24	0.2118	0.0863
303.09	0.2667	0.1910	343.18	0.3186	0.1269
303.01	0.3975	0.2571	343.23	0.5236	0.1846
303.00	0.9242	0.5031	343.23	1.1982	0.3719
303.04	0.9392	0.5104	343.21	1.2994	0.3892
303.03	1.3353	0.6642	343.20	1.8465	0.5068
323.08	0.1557	0.0854	363.24	0.1876	0.0606
323.09	0.1950	0.1044	363.22	0.2249	0.0727
323.03	0.2964	0.1545	363.13	0.3356	0.1068
323.07	0.4668	0.2176	363.33	0.5688	0.1593
323.07	1.0857	0.4308	363.31	1.2811	0.3217
323.07	1.1426	0.4450	363.33	1.4194	0.3419
323.07	1.6501	0.5780	363.33	1.9742	0.4461

$\ln(H_{2,1}/\text{MPa}) = (2.067 \pm 0.011) - (1523 \pm 33)[1/(T/\text{K}) - 1/333.15]$

Solvent Chem. Abstr. Name: 2,2-bis[(1-oxononyl)oxylmethyl]-1,3-propanediyl ester of nonanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant, and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (>0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Materials:
(1) 1,1,1-Trifluoroethane. DuPont de Nemours, Dodrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetranonanate. Synthesized from pentaerythriiol and nonanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%.

Estimated Error:
Uncertanties in T and p not given in this paper. $\delta H/H < 0.02$ at low pressure: <0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]J. Chem. Eng. Data **44**, 823 (1999).

3.14. 1,1-Difluoroethane

Components:
(1) 1,1-Difluoroethane; $C_2H_4F_2$; [75-37-6]
(2) Water; H_2O; [7732-16-5]

Evaluators:
H. Lawrence Clever,
Emory University, Atlanta, GA 30322
June 2003

Evaluation

An evaluation of the solubility of 1,1-difluoroethane in water from 273.15 K to 338.19 K at a partial pressure of 0.101325 MPa.

Three papers report the solubility of 1,1-difluoroethane in water. Manheimer[1] reports one value at 273.15 K; Makitra *et al.*[2] report measurements at four partial pressures from 0.013 MPa to 0.0973 MPa at four temperatures from 283.2 K to 313.2 K and Zheng *et al.*,[3] report two values at each of three temperatures. None of the papers report the mole fraction solubility at a partial pressure of 0.101325 MPa. The evaluator calculated the mole fraction solubility at a partial pressure of 0.101325 MPa from the data in the papers assuming ideal gas behavior and Henry's law. The results are shown in Table 12.

The paper of Zheng, Guo, and Knapp[3] gives values of the Henry's constant based on just one measurement of partial pressure and solubility. The values above in () are calculated from the author's Henry's constants. The evaluator calculated the first value in the column assuming an ideal gas and Henry's law.

All of the values are classed as tentative, but no equation of tentative values is given. The user may make his or her own choices.

References

[1]M. Mannheimer, Chemist-Analyst **45**, 8–10 (1956).

[2]R. G. Makitra, T. I. Politanskaya, F. B. Moin, and G. P. Kostyak, Deposited Document (1982) VINITI 1733–82.

[3]D.-Q. Zheng, T.-M. Guo, and H. Knapp, Fluid Phase Eq. **129**, 197–209 (1997).

TABLE 12. Comparisons of mole fraction solubility of 1,1-di-fluoroethane in water at several temperatures and a partial pressure of 0.101325 MPa from three papers

Temperature (T/K)	Mannheimer[1] 10^4x_1	MPMK[2] 10^4x_1	ZGK[3] 10^4x_1
273.15	15.		
278.19			18.3 (18.9)
283.15		9.68	
293.15		7.79	
303.15		6.03	
308.13			6.10 (6.78)
313.15		5.10	
338.19			2.50 (3.70)

Components:
(1) 1,1-Difluoroethane; $C_2H_4F_2$; [75-37-6]
(2) Water: H_2O; [7732-18-5]

Original Measurements:
M. Mannheimer, Chemist-Analyst **45**, 8–10 (1956).

Variables:
T/K = 273
p_1 /KPa = 101

Prepared By:
H. L. Clever

Experimental Values

The aqueous solution in equilibrium with CH_3CHF_2 gas at 0 °C mmHg is 99.46 wt % water.

The compiler esitmates the mole fraction solubility of CH_3CHF_2 in water under these conditions as $x_1 = 0.0015$.

The author credits the information to unpublished data courtesy of the General Chemical Division, Allied Chemical and Dye Corporation.

Auxiliary Information

Method/Apparatus/Procedure:
No information.

Source and Purity of Material:
(1) 1,1-Difluoroethane.
(2) Water.
Nothing specified for either component.

Estimated Error:
$\delta x_1 / x_1 = \pm 0.10$ (Compiler).

Components:
(1) 1,1-Difluoroethane; $C_2H_4F_2$; [75-37-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, and G. P. Kostyk, Dep. Document (1982), VINITI 1733–82.

Variables:
T/K = 283.2–313.2
p_1 /MPa = 0.0133–0.0973

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

Temperature		Pressure		Mol Fraction
(t/°C)	(T/K)	(p_1 /mmHg)	(P_1 /MPa)	$10^4 x_1$
10	283.2	100	0.0133	1.318
		300	0.0400	3.974
		500	0.0667	6/584
		730	0.0973	9.293
20	293.2	100	0.0133	1.048
		300	0.0400	3.144
		500	0.0667	5.238
		730	0.0973	7.480
30	303.2	100	0.0133	0.796
		300	0.0400	2.461
		500	0.0667	4.126
		730	0.0973	5.789
40	313.2	100	0.0133	0.701
		300	0.0400	2.102
		500	0.0667	3.503
		730	0.0973	4.903

The Kelvin temperatures and the MPa pressure values were added by the compiler (HLC).
The authors give a heat of sorption of 3.70 kcal mol^{-1} (15.5 kJ mol^{-1}).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is described in an earlier paper.[1]
The authors state the sorption obeys Henry's law.

Source and Purity of Materials:
(1) 1,1-Difluoroethane. Source not given. Stated to be chromatographically pure.
(2) Water. Distilled.

Estimated Error:
Nothing specified by authors.

References:
[1]G. E. Braude, I. L. Leites, and I. Z. Dedova, Khim. Prom. (4), 232 (1961).

Components:
(1) 1,1-Difluoroethane; $C_2H_4F_2$; [75-37-6]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
D.-Q. Zheng, T.-M. Guo, and H. Knapp, Fluid Phase Eq. **129**, 197–209 (1997).

Variables:
T/K = 278.12–338.19
p/MPa = 0.03664–0.08925

Prepared By:
H. L. Clever

Experimental Values

The solubility of $C_2H_4F_2$ in water and aqueous NaCl

T/K	p/MPa	Sodium Chloride (n_2 /mol mol^{-1})	Mole Fraction $10^4 x_1$	Henry's Constant ($H_{1,s}$ /MPa)
278.19	0.03667	0.00	6.60	53.84
278.19	0.03724		6.74	53.53
308.13	0.06161		3.71	149.3
308.13	0.06236		3.75	149.8
338.19	0.07926		1.96	275.9
338.19	0.07992		1.97	271.5
278.16	0.03998	0.0121	6.50	59.66
278.16	0.04030		6.60	59.28
308.10	0.06439		3.50	166.0
308.10	0.06581		3.56	167.3
338.16	0.08089		1.80	308.3
338.16	0.08319		1.85	312.3
278.14	0.04262	0.0295	5.96	69.92
278.14	0.04290		5.97	69.33
308.16	0.06576		3.16	189.1
308.16	0.06851		3.30	188.8
338.14	0.08322		1.63	357.0
338.14	0.08364		1.66	352.8
278.12	0.05111	0.0564	5.23	95.11
278.12	0.05171		5.29	95.13
308.16	0.07288		2.60	257.3
308.16	0.07484		2.65	259.0
338.09	0.08694		1.27	494.8
338.07	0.08925		1.29	504.7

The above NaCl mol ratios correspond to 0.672, 1.64, and 3.13 mol kg^{-1} (molality), respectively.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental apparatus consists of a degassing system and a gas absorption unit. The water and NaCl solutions were degassed by vacuum with stirring until the vapor pressure of the solvent was reached. The degassed solvent was transferred to an evacuated glass cell and weighed to 0.0001 g. The cell was thermostated and the adsorption apparatus evacuated before the gas was admitted. The solvent was stirred constantly. When the system T and p were constant, the equilibrium state was established.

Source and Purity of Materials:
(1) 1,1-Difluoroethane or R-152a. Hoechst. Purity stated to be 99.0 volume %.
(2) Sodium chloride. Merck. Laboratory grade.
(3) Water. Deionized at the Institute.

Estimated Error:
δT/K = ±0.1
$\delta p/p$ = ±0.001
$\delta x_1/x_1$ = ±0.005
(Compiler's estimates).

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **74**, 426–428 (1996).

Variables:
T/K = 303.15–343.15
p_1 /kPa = 10–50

Prepared By:
H. L. Clever

Experimental Values

T/K	Henry's Constant Isochoric Method (He/MPa)	Henry's Constant GLC Method (He/MPa)	δHe/MPa (%)
303.15	2.29	2.45	7.1
323.15	3.11	3.30	6.2
343.15	4.04	4.30	6.7

Henry's constant He/MPa = $\lim_{x_1 \to 0} (f_1$ /MPa$)/x_1$

Isochoric Method. At equilibrium $f_1^l = f_1^v = \varphi_1{}^v y_1 p$. Hexadecane has negligible vapor pressure so y_1 can be taken equal to unity. The gas phase fugacity coefficient is calculated with an equation of state. As the equilibrium pressures is only 10–50 kPa, $\varphi_1{}^v$ is close to unity (0.994–0.998).

$\delta He = (|He_{isochor} - He_{GLC})/He_{isochor}$. He is the authors symbol for the Henry's constant.

Auxiliary Information

Method/Apparatus/Procedure:
Two methods were used.
The Isochoric Method. The apparatus is the same as that used by Maassen *et al.*[1] The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification section of a vacuum pump attached to the equilibrium cell with a magnetic stirrer; a liquid-bath thermostat surrounding the equilibrium cell and an air-bath with the calibrated gas bottle and a pressure transducer.
The GLC Method. The apparatus and procedure are the same as described by Zuliani *et al.*[2] The hexadecane is deposited *in situ* on the column as the stationary phase. The column is flushed with N_2 until a constant weight of column is reached; a steady state is attained; and the solute is injected. For both methods see the paper for more details.

Source and Purity of Materials:
(1) Difluoroethane. No source specified. Stated to be of 99.4% purity.
(2) Hexadecane. No source specified. Stated to be of over 99% purity.

Estimated Error:
$\delta T/T = \pm 0.00016$ Isochoric Method
$\delta p/p = \pm 0.0015$ Isochoric Method
$\delta He/He = < \pm 0.02$ Isochoric Method
$\delta He/He = \pm 0.05$ GLC Method

References:
[1]S. Massen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]M. A. Zuliani, A. Barreau, J. Vidal, P. Alessi, and M. Fermeglia, Fluid Phase Eq. **82**, 141 (1992).

Components:
(1) 1,1-Difluoroethane or HFCl152a; $C_2H_4F_2$; [75-37-6]
(2) Hexadecane; $C_{16}H_{34}$; [544-76-3]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 293.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution $-\gamma^\infty$
293.15	1.82	4.04
303.15	2.27	3.86
323.15	3.10	3.31
343.15	4.03	2.93
363.15	5.06	2.68

Henry's constant He/MPa = $\lim_{x_1 \to 0} (f_1$ /MPa$)/x_1$

Isochoric Method. At equilibrium $f_1{}^l = f_1{}^v = \varphi_1{}^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three values below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1{}^\infty = (He_{1,2})/f^{*l}{}_1$. It is not calculated for the solute when at temperatures above the critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainles steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1-Difluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Hexadecane. Lancaster Synthesis, Morecame, England. Said to be of 99% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
2 W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) 2,6,10-14-Tetramethylpentadecane; $C_{19}H_{40}$; [1921-70-6]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 293.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution $-\gamma^{\infty}$
293.15	1.49	3.32
303.15	1.80	3.05
323.15	2.47	2.64
343.15	3.24	2.35
363.15	4.09	2.17

Henry's constant $He/\text{MPa} = \lim_{x_1 \to 0} (f_1\ /\text{MPa})/x_1$

Isochoric Method. At equilibrium $f_1{}^l = f_1{}^v = \varphi_1{}^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three values below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1{}^{\infty} = (He_{1,2})/f^{*l}{}_1$. It is not calculated for the solute when at temperatures above the critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1-Difluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) 2,6,10,14-Tetramethylpentadecane. Sigma Chemical Co., St. Louis, MO. Said to be of 99% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Massen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. A. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Eicosane; $C_{20}H_{42}$; [112-95-8]

Original Measurements:
Å. Wahlström and L. Vamling, Can. J. Chem. Eng. **75**, 544–550 (1997).

Variables:
T/K = 323.15–363.15
p_1 /MPa = 0.05–2

Prepared By:
H. L. Clever

Experimental Values

Henry's constant of 1,1-difluoroethane in eicosane between 323.15 K and 363.15 K

T/K	Henry's Constant (He/MPa)	Activity Coefficients At Infinite Dilution-γ^{∞}
323.15	2.72	2.90
343.15	3.51	2.55
363.15	4.29	2.28

Henry's constant: $He/\text{MPa} = \lim_{x_1 \to 0} (f_1\ /\text{MPa})/x_1$

Isochoric Method. At equilibrium, $f_1^l = f_1^v = \varphi_1^v y_1 p$. The gas phase fugacity coefficient is calculated with an equation of state. Henry's constant is calculated from at least three measurements below 0.28 MPa. The activity coefficient at infinite dilution is calculated from $\gamma_1^{\infty} = (He_{1,2})/f_1^{*l}$. It is not calculated for the solute at temperatures above the critical temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The Isochoric Method. The apparatus is essentially the same as that used by Maassen *et al.*[1] and Metzer *et al.*[2] A major change is replacement of glass by stainless steel which allows pressures up to 3 MPa. The amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas bottle of known volume, observed during the absorption of the gas. The apparatus consists of a degasification system of a vacuum pump attached through a liquid N_2 trap to the equilibrium cell with a magnetic stirrer. A liquid bath thermostat surrounds the equilibrium cell. A second liquid bath thermostat contains the calibrated gas bottle and an air bath thermostat is used for other connecting parts and a pressure transducer.

Source and Purity of Materials:
(1) 1,1,1,2-Difluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Eicosane. Sigma Chemical Co., St. Louis, MO. Stated to be of 98% pure.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p/p = \pm 0.001$
δHe/He = $< \pm 0.02$ at low pressure;
$= < \pm 0.03$ at high pressure.

References:
[1]S. Maassen, A. Reichel, and H. Knapp, Fluid Phase Eq. **82**, 71 (1993).
[2]W. M. Melzer, F. Schrödter, and H. Kapp, Fluid Phase Eq. **49**, 167 (1989).

Components:
(1) 1,1 Difluoroethane or HFC152a; $C_2H_4F_2$; [75-46-7]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283–313.29
p_1 /MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

The solubility of 1,1-difluoroethane in methanol from 283.15 K to 313.29 K at a partial pressure of 0.101325 MPa

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant $[H_{1,2}$ /MPa$=(p_1$ /MPa$)/x_1]$
283.18	0.0603	0.9279	1.55
293.02	0.0420	0.8733	2.10
303.17	0.0261	0.8176	3.17
313.29	0.0146	0.7002	4.87

The author approximated the 1,1-difluoroethane partial pressure as p_1 /MPa $=(p_t$ /MPa$)y_1=0.1031y_1$.
They fitted the Henry's constant to the equation:
$\ln(H_{1,2}$ /MPa$) = -487.045 + 18\,819.437/(T/\mathrm{K}) + 74.57 \ln(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions. Measurements were repeated three times.

Source and Purity of Materials:
(1) 1,1-Difluoroethane. Daikin Industries, Ltd. Stated to be greater than 99.8% pure.
(2) Methanol. Wake Pure Chemicals, Ltd. Stated to be 99.8% pure.

Estimated Error:
δT/K $= \pm 0.1$
$\delta x_1/x_1 = < \pm 0.02$ for the liquid phase
$= \pm 0.005$ for the vapor phase.
$\delta H/H = \pm 0.025$.

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Methanol; CH_4O; [67-56-1]

Original Measurements:
R. Kato and H. Nishiumi, J. Chem. Eng. Data **47**, 1140–1144 (2002).

Variables:
T/K = 303.0–323.0
p /kPa = 47.7–94.3

Prepared By:
H. L. Clever

Experimental Values

The solubility of 1,1-difluoroethane in methanol from 303.0 K to 323.0 K

T/K	p/kPa	Liquid Mol Fraction	Vapor Mol Fraction	Henry's Constant (H/MPa)
303.0	47.7	0.01080	0.521	2.40
	48.3	0.01060	0.521	
308.0	58.9	0.00940	0.473	2.90
	55.1	0.00820	0.443	
313.0	73.2	0.00960	0.452	3.40
	69.6	0.00890	0.429	
	69.1	0.00850	0.416	
313.0	74.8	0.00740	0.374	3.69
	73.9	0.00750	0.367	
323.0	94.3	0.00910	0.391	4.09
	89.1	0.00770	0.358	

The authors fit the Henry constants to the equation: $\ln(H/\mathrm{MPa}) = 32.95 - 3663/(T/\mathrm{K}) - 3.493\ln(T/\mathrm{K})$.
At 303 K and 101 kPa the mole fraction of CH_2F_2 in methanol is 0.0423 and the entropy of solution is -68.90 J K^{-1} mol^{-1}.

Auxiliary Information

Method/Apparatus/Procedure:
The method was head space gas chromatography. The HS-40 Perkin-Elmer head space autosampler gas chromatograph was used. Equilibrium cells were 22 mL glass vials. The autosampler, in a constant temperature bath, could contain up to 13 vials. The solvent was weighed in a glass ampule and placed in a sample vial; the fluorocarbon was charged into the vial and weighed. The fluorocarbon weight and the air weight replaced by fluorocarbon were used to determine the overall composition. The solvent ampule was broken and the system equilibrated for 3 h, the headspace vapor was injected for 3 s into the gas chromatograph by the auto-sampler program. Details of the calculation are in the paper.

Source and Purity of Materials:
(1) 1,1-difluoroethane. Toei Chem. Ind. (Tokyo). Purity stated to be 99.9%, used as received.
(2) Methanol. Kanto Chem. Ind. (Tokyo). Purity stated to be 99.5%, used as received.

Estimated Error:
δT/K $= \pm 0.1$
$\delta x_1/x_1 = \pm 0.008$ av.; ± 0.022 max.
$\delta y_1/y_1 = \pm 0.008$ av.; ± 0.021 max.

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measuremens:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.18–313.1
p_t/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

The solubility of 1,1-difluoroethane in ethanol from 283.18 K to 313.1 K at a partial pressure of 0.101325 MPa

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant ($H_{1,2}$/MPa = (p_1/MPa)/x_1)
283.18	0.0611	0.9708	1.61
292.94	0.0465	0.9460	2.06
303.	0.0348	0.8976	2.61
313.1	0.0253	0.8228	3.29

The authors approximated the 1,1-difluoroethane partial pressure as p_1/MPa = (p_t/MPa)y_1 = 0.1013y_1.

They fitted the Henry's constants to the equation:

$$\ln(H_{1,2}/\mathrm{MPa}) = -18.866 - 925.958(T/\mathrm{K}) + 4.005\ \ln(T/\mathrm{K}).$$

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath.
The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions. Measurements were repeated three times.

Source and Purity of Materials:
(1) 1,1-Difluoroethane. Daikin Industries, Ltd. Stated to be greater than 99.8% pure.
(2) Ethanol. Wake Pure Chemicals, Ltd. Stated to be 99.8% pure.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = < ±0.02 for the liquid phase
= ±0.005 for the vapor phase.
$\delta H/H$ = ±0.025.

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Ethanol; C_2H_6O; [64-17-5]

Original Measurements:
R. Kato and H. Nishiumi, J. Chem. Eng. Data **47**, 1140–1144 (2002).

Variables:
T/K = 308.0–323.0
p/kPa = 35.6–78.6

Prepared By:
H. L. Clever

Experimental Values

The solubility of difluoroethane in ethanol from 303.0 K to 323.0 K

T/K	p/kPa	Liquid Mol Fraction $-x_1$	Vapor Mole Fraction $-y_1$	Henry's Constant (H/MPa)
303.0	43.8	0.01410	0.763	2.35
	35.6	0.01100	0.727	
308.0	54.5	0.01380	0.708	2.76
	47.5	0.01170	0.668	
313.0	56.2	0.01240	0.654	2.96
	58.0	0.01280	0.660	
	49.8	0.01060	0.620	
323.0	71.2	0.01070	0.559	3.76
	78.6	0.01230	0.593	

The authors fit the Henry constants to the equation $\ln(H/\mathrm{MPa}) = 32.50 - 3357/(T/\mathrm{K}) - 3.598\ \ln(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
The method was head space gas chromatography. The HS-40 Perkin-Elmer head space autosampler gas chromatograph was used. Equilibrium cells were 22 mL glass vials. The autosampler, in a constant temperature bath, could contain up to 13 vials. The solvent was weighed in a glass ampule and placed in a sample vial; the fluorocarbon was charged into the vial and weighed. The fluorocarbon weight and the air weight replaced by fluorocarbon were used to determine the overall composition. The solvent ampule was broken and the system equilibrated for 3 h, the headspace vapor was injected for 3 s into the gas chromatograph by the auto-sampler program. Details of the calculation are in the paper.

Source and Purity of Materials:
(1) 1,1-Difluoroethane. Toei Chem. Ind. (Tokyo). Purity stated to be 99.9%, used as received.
(2) Ethanol. Kanto Chem. Ind. (Tokyo). Purity stated to be 99.5%, used as received.

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.008 av.; ±0.022 max.
$\delta y_1/y_1$ = ±0.008 av.; ±0.021 max.

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) 2-Propanol; C_3H_8O; [67-63-0]

Original Measurements:
M. Takenouchi, R. Kato, and H. Nishiumi, J. Chem. Eng. Data **46**, 746–749 (2001).

Variables:
T/K = 283.18–313.3
p_t /MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Solubility of 1,1-difluoroethane in 2-propanol from 283.18 K to 313.K at a partial pressure of 0.1013 MPa

T/K	Mole Fraction Liquid x_1	Mole Fraction Vapor y_1	Henry's Constant $[H_{1,2}$ /MPa = $(p_1$ /MPa$)/x_1]$
283.18	0.0590	0.9758	1.67
293.06	0.0438	0.9565	2.21
293.06	0.0438	0.9565	2.21
303.15	0.0338	0.9269	2.78
313.3	0.0258	0.8614	3.38

The second 293.06 K entry may be an error in the original paper.

The authors approximated the 1,1-difluoroethane partial pressure as p_1 /MPa = $(p_t$ /MPa$)y_1 = 0.1013y_1$.

They fitted the Henry's constants to the equation: $\ln(H_{1,2}$ /MPa$) = 174.993 - 9500.782(T/\mathrm{K}) - 24.96\ln(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
An equilibrium cell equipped with sampling septums for microsyringes to sample both liquid and vapor phases, a ball filter to introduce the gas and agitate the solution and a thermometer probe was in a thermostated water bath. The gas was blown into the alcohol through the ball filter to dissolve and to agitate the solution. The pressure was maintained at atmospheric pressure, 0.1013 MPa. The time required to reach equilibrium was not mentioned. At equilibrium the vapor phase was sampled with a 2.5 mL warmed syringe containing 0.5 mL of helium gas to prevent alcohol condensation. The liquid phase was sampled with a 10 μL microsyringe. The samples were injected into a gas chromatograph with a TCD detector to determine the liquid and vapor phase compositions. Measurements were repeated three times.

Source and Purity of Materials:
(1) 1,1-Difluoroethane. Daikin Industries, Ltd. Stated to be 99.8% pure.
(2) 2-Propanol. Wake Pure Chemicals, Ltd. Stated to be 99.5% pure.

Estimated Error:
δT/K = ±0.1
δ_1 / x_1 = < ±0.02 for the liquid phase
= ±0.005 for the vapor phase.
$\delta H/H$ = ±0.025.

Components:
(1) 1,1-Difluoroethane; $C_2H_4F_2$; [75-37-6]
(2) 2-Propanone or acetone; C_3H_6O; [67-64-1]

Original Measurements:
T. S. Siribaev, E. F. Nakhodzhaev, A. A. Yul'chibaev, and Kh. U. Usamnov, Nauch. Tr. Tashkent Un-t. (No. 462), 103–105 (1974).

Variables:
T/K = 283.2–313.2
p_1 /MPa = 0.203–0.068

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

Temperature		Pressure		Solubility
(t/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	S/cm^3 (STP) g^{-1}
10	283.2	2	0.203	667
20	293.2	2	0.203	350
30	303.2	2	0.203	142
		4	0.405	517
40	313.2	2	0.203	83
		4	0.405	300
		6	0.608	583

The compiler (YPY) took the values from graphs in the original paper. The compiler (HLC) added the Kelvin temperatures and the MPa pressure values. The system appears to be quite nonideal. Henry's law is not obeyed.

Auxiliary Information

Method/Apparatus/Procedure:
Volumetric method. The apparatus is described in an earlier paper.[1]

Source and Purity of Materials:
(1) 1,1-Difluoroethane. Nothing specified.
(2) Acetone. Nothing specified.

Estimated Error:
Nothing specified by authors.

References:
[1]E. R. Shenderei, Ya. D. Zel'vensskii, and F. P. Ivanovskii, Khim. Prom. (5), 370 (1960).

Components:
(1) 1,1-Difluoroethane; $C_2H_4F_2$; [75-37-6]
(2) 1,4-Dioxane; C4H8O2; [123-91-1]

Original Measurements:
E. F. Narkhodzhaev, T. S. Sirlibaev, A. A. Yulchibaev, and Kh. U. Usamnov, Uzb. Khim. Zh. **19**(3), 19–20 (1975).

Variables:
T/K=285.2–303.2
p_1 /kPa=11.2–89.0

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

Temperature (t/°C)	Temperature (T/K)	Pressure (p_1 /atm)	Pressure (p_1 /MPa)	Mol Fraction x_1
12	285.2	84	11.20	0.014
		161	21.46	0.031
		258	34.40	0.054
		340	45.33	0.074
		461	61.46	0.105
		541	72.13	0.127
		633	84.39	0.152
20	293.2	99	13.20	0.011
		193	25.73	0.027
		316	42.13	0.054
		409	54.53	0.071
		483	64.39	0.084
		592	78.93	0.084
		632	84.26	0.112
30	303.2	126	16.80	0.009
		228	30.40	0.022
		359	47.86	0.039
		469	62.53	0.052
		550	73.33	0.063
		611	81.46	0.072
		660	87.99	0.079

The compiler (HLC) added the Kelvin temperatures and the kPa pressure values. The authors conclude Henry's law is obeyed.

Auxiliary Information

Method/Apparatus/Procedure:
Static method. The apparatus is described in an earlier paper.[1]

Source and Purity of Material:
(1) 1,1-Difluoroethane. Nothing specified.
(2) 1,4-Dioxane. Nothing specified.

Estimated Error:
Nothing specified by authors.

References:
[1]G. E. Braude and S. F. Shahova, Khim. Prom. (3), 177 (1961).

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Pentaerythitol tetrapentanonate ester; $C_{25}H_{44}O_8$; [15834-04-5] *Chem. Abstr.* name: Pentanoic 2,2-*bis*[(1-oxypentyl)oxylmethyl]-1,3-propanediyl ester.

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823–828 (1999).

Variables:
T/K=303.15–363.15
p_1 /MPa=0.05–1.9

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1 /MPa	Mol Fraction x_1
303.16	0.0585	0.1167	343.15	0.1101	0.0883
303.15	0.0770	0.1532	343.15	0.1441	0.1186
303.16	0.1552	0.2900	343.17	0.2958	0.2357
303.15	0.2158	0.3764	343.15	0.4174	0.3097
303.15	0.2681	0.4497	343.16	0.5405	0.3820
303.15	0.3800	0.5824	343.17	0.7473	0.4845
323.26	0.0844	0.1023	363.26	0.1346	0.0753
323.26	0.1103	0.1360	363.23	0.1758	0.1026
323.28	0.2250	0.2636	363.22	0.3635	0.2083
323.26	0.3157	0.3445	363.24	0.5144	0.2744
323.25	0.4009	0.4183	363.26	0.6753	0.3434
323.26	0.5647	0.5389	363.24	0.9043	0.4264

Henry's constant was calculated for the 8 points at pressures below 0.24 MPa and fitted to the equation, $\ln(He_{1,2}/\mathrm{MPa}) = \ln(0.979 \pm 0.017) - (2277 \pm 86)[1/(T/\mathrm{K}) - 1/333.15]$. The CH_2F_2 activity coefficients at infinite dilution are: $(T/\mathrm{K})/\gamma^{\infty}$ 303.2/0.84; 323.2/0.86; 343.2/0.88; 363.2/0.91.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from pressure changes in a gas system of known volume, observed during the absorption of the gas. The apparatus consists of three sections. (*i*) A liquid bath thermostat 1 containing the equilibrium cell with a magnetic stirrer; (*ii*) liquid bath thermostat 2 with a gas bottle of calibrated volume; (*iii*) an air bath thermostat with a pressure transmitter and connections between the first two sections and to a gas storage and a vacuum pump. More details of the apparatus, the experimental technique and the treatment of the data are in an earlier paper of the authors.[1]

Source and Purity of Material:
(1) 1,1-Difluoroethane. DuPont de Nemours, Dordrecht Works. Stated to be 99.9% pure.
(2) Pentaerythritol tetrapentanonate ester. Synthesized[2] by a reaction between valeric acid and pentaerythritol catalyzed with p-toluenesulfonic acid in a p-xylene solvent. The product was vacuum distilled. NMR and IR results gave a purity >95%.

Estimated Error:
$\delta T/T = \pm 0.00016$
$\delta p_1/p_1 = \pm 0.001$
$\delta He/He = < \pm 0.02$ at low pressures,
$= < \pm 0.03$ at high pressures.

References:
[1]Å. Wahlstrom and L. Vamling, Can. J. Chem. Eng. **75**, 544 (1997).
[2]K. D. Black and F. D. Gunstone, Chem. Phys. Lipids **56**, 169 (1990).

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Pentaerythritol tetra-2-ethylbutanoate; $C_{29}H_{52}O_8$; [139611-32-8]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 323.12–363.29
p_1 /MPa = 0.0964–0.9074

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1 /MPa	Mol Fraction x_1
			343.29	0.1219	0.1074
	The		343.28	0.1273	0.1142
	solvent		343.26	0.1407	0.1244
303.15	is a solid		343.29	0.3793	0.2978
	at this		343.28	0.5036	0.3766
	temperature		343.28	0.7400	0.5021
323.13	0.0964	0.1256	363.28	0.1446	0.0915
323.13	0.1023	0.1345	363.29	0.1489	0.0964
323.12	0.1091	0.1447	363.28	0.1689	0.1064
323.14	0.2937	0.3387	363.27	0.4537	0.2585
323.12	0.3809	0.4173	363.26	0.6157	0.3394
323.12	0.5506	0.5485	363.17	0.9074	0.4513

$$\ln(H_{2,1}/\text{MPa}) = (0.909 \pm 0.009) - (2114 \pm 64)[1/(T/\text{K}) - 1/333.15]$$

Solvent Chem. Abstracts Name: 2,2-bis[(2-ethyl-1-oxobutoxy)methyl]-1.3-propanediyl ester of 2-ethyl butanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant, and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) Difluoromethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylbutanoate. Synthesized from pentaerythriiol and 2-ethyl-butanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%. Melting point 310–312 K.

Estimated Error:
Uncertanies in T and p not given in this paper.
$\delta H/H < 0.02$ at low pressure; < 0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Pentaerythritol tetra-2-ethylhexanoate; $C_{37}H_{68}O_8$; [7299-99-2]

Original Measurements:
Å. Wahlstrom and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 303.11–363.31
p_1 /MPa = 0.0751–0.8732

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1 /MPa	Mol Fraction x_1
303.11	0.0751	0.1576	343.21	0.1242	0.1163
303.18	0.0842	0.1739	343.26	0.1388	0.1294
303.18	0.1007	0.2053	343.26	0.1681	0.1534
303.19	0.2618	0.4544	343.31	0.4371	0.3435
303.16	0.4006	0.5865	343.15	0.7368	0.4817
323.04	0.1000	0.1367	363.18	0.1451	0.0990
323.10	0.1116	0.1516	363.29	0.1626	0.1100
323.12	0.1347	0.1794	363.26	0.1971	0.1307
323.14	0.3552	0.3999	363.31	0.5015	0.2930
323.28	0.5739	0.5388	363.24	0.8732	0.4221

$$\ln(H_{2,1}/\text{MPa}) = (0.873 \pm 0.006) - (2051 \pm 31)[1/(T/\text{K}) - 1/333.15]$$

Solvent Chem. Abstracts Name: 2,2-bis[(2-ethyl-1-oxohexyl)oxylmethyl]-1,3-propanediyl ester of 2-ethyl hexanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) 1,1-Difluoroethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetr-2-ethylhexanoate. Synthesized from pentaerythriiol and 2-ethyl-hexanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >90%. Contains 5%–10% di- and tri-esters.

Estimated Error:
Uncertanies in T and p not given in this paper.
$\delta H/H < 0.02$ at low pressure; < 0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem Eng. **75**, 544 (1997);
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

Components:
(1) 1,1-Difluoroethane or HFC152a; $C_2H_4F_2$; [75-37-6]
(2) Pentaerythritol tetrananoate; $C_{41}H_{76}O_8$; [14450-05-6]

Original Measurements:
Å. Wahlström and L. Vamling, J. Chem. Eng. Data **45**, 97–103 (2000).

Variables:
T/K = 303.11–363.24
p_1 /MPa = 0.1131–1.0220

Prepared By:
H. L. Clever

Experimental Values

T/K	p_1 /MPa	Mol Fraction x_1	T/K	p_1 /MPa	Mol Fraction x_1
303.15	0.1131	0.2286	343.26	0.1693	0.1575
303.11	0.1190	0.2361	343.21	0.1780	0.1627
303.11	0.1335	0.2604	343.21	0.2001	0.1815
303.17	0.1821	0.3276	343.26	0.3139	0.3578
303.18	0.3287	0.5096	343.26	0.5638	0.4071
303.16	0.3418	0.5214	343.22	0.6276	0.4344
303.16	0.4642	0.6481	343.25	0.8665	0.5472
323.10	0.1438	0.1909	363.24	0.1891	0.1317
323.05	0.1513	0.1970	363.20	0.1996	0.1342
323.05	0.1699	0.2185	363.17	0.2238	0.1512
323.09	0.2492	0.2930	363.22	0.3722	0.2245
323.09	0.4519	0.4607	363.21	0.6539	0.2681
323.09	0.4896	0.4810	363.22	0.7507	0.3893
323.09	0.6704	0.6034	363.22	1.0220	0.4893

$$\ln(H_{2,1}/\text{MPa}) = (0.882 \pm 0.009) - (1958 \pm 52)[1/(T/\text{K}) - 1/333.15]$$

Solvent Chem. Abstr. Name: 2,2-bis[(1-oxononyl)oxylmethyl]-1,3-propanediyl ester of nonanoic acid.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique is an isochoric one where the amount of gas absorbed in a known quantity of liquid solvent is calculated from the pressure change in a gas system of known volume, observed during the absorption of the gas. The experimental equipment and its calibration are described in an earlier paper.[1] The calculations of absorbed gas, Henry's constant and the activity coefficient at infinite dilution are described in another paper.[2] All the experimental data are correlated with an extended Flory-Huggins model. The model is based on equality of vapor and liquid fugacities. The low pressure (<0.34 MPa) experimental data are correlated with the Henry's constant equation below the table.

Source and Purity of Material:
(1) 1,1,-Difluoroethane. DuPont de Nemours, Dordrecht Works, The Netherlands. Stated to be 99.9%.
(2) Pentaerythritol tetranonanoate. Synthesized from pentaerythriiol and nonanoic acid catalyzed by toluenesulfonic acid in p-xylene solvent. The product was washed, dried, and vacuum distilled. NMR and IR gave a purity of >95%.

Estimated Error:
Uncertanies in T and p not given in this paper.
$\delta H/H < 0.02$ at low pressure; < 0.03 at high.

References:
[1]Å. Wahlström and L. Vamling, Can. J. Chem Eng. **75**, 544 (1997).
[2]Å. Wahlström and L. Vamling, J. Chem. Eng. Data **44**, 823 (1999).

3.15. Fluoroethane

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Heptane; C_7H_{16} ; [142-85-5]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983). J. Appl. Chem. USSR (Engl. Trans.) **56**, 2048–2051 (1983).

Variables:
T/K = 253.2, 273.2, and 293.2
p_1 /kPa = 13.3–97.3 (100–730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values
Solubility of fluoroethane in heptane from 253.2 K to 293.2 K as a function of partial pressure

T/K	p_1 /mmHg	p_1 /kPa	Mole Fraction x_1	Volume Absorbed (V/cm^3)
253.2	100	13.3	0.03408	5.0
	300	40.0	0.07808	12.0
	500	66.7	0.16989	29.0
	730	97.3	0.31447	65.0
273.2	100	13.3	0.02549	4.0
	300	40.0	0.06139	10.0
	500	66.7	0.09473	16.0
	730	97.3	0.15008	27.0
293.2	100	13.3	0.01204	2.0
	300	40.0	0.02611	4.4
	500	66.7	0.04870	8.4
	730	97.3	0.10377	19.0

The pressures appear to be the partial pressure of fluoroethane.
The compiler added the kPa pressure values.
The volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 of solvent and then adjusted to 1 atm pressure.
The authors give the enthalpy of solution as ΔH/kcal mol^{-1} = −4.10.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) Tetrahydrofuran.
Described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Benzene; C_6H_6; [71-43-2]
(2) Methylbenzene or toluene; C_7H_8; [108-88-3]
(2) 1,4-Dimethylbenzene; C_8H_{10}; [106-42-3]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983). J. Appl. Chem. USSR (Engl. Transl.) **56**, 2048–2051 (1983).

Variables:
T/K = 293.2
p_1 /kPa = 97.3 (730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in several aromatic hydrocarbons at 293.2 K and a partial pressure of 97.3 kPa.

Solvent	T/K	p_1 /mmHg	Mole Fraction (x_1)	Volume Absorbed (V/cm^3)
Benzene	293.2	730	0.05781	16.6
Methylbenzene	293.2	730	0.14100	34.6
1,4-Dimethyl-benzene	293.2	730	0.11770	26.8

The 730 mmHg (97.3 kPa) appears to be the partial pressure of the fluoroethane. Volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 solvent and then adjusted to 1 atm pressure

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) The aromatic hydrocarbons.
Described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) 2-Propanone or acetone; C_3H_6O; [67-64-1]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983). J. Appl. Chem. USSR
(Engl. Trans.) **56**, 2048–2051 (1983).

Variables:
T/K = 253.2, 273.2, and 293.2
p_1 /kPa = 13.3–97.3 (100–730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in 2-propanone (acetone) at temperatures of 253.2 K, 273.2 K, and 293.2 K, and partial pressures from 13.3–97.3 kPa

T/K	p_1 /mmHg	p_1 /kPa	Mole Fraction-x_1	Volume Absorbed (V/cm^3)
253.2	100	13.3	0.05979	18.0
	300	40.0	0.20723	74.0
	500	66.7	0.26104	100.0
	730	97.3	0.46897	250.0
273.2	100	13.3	0.00973	3.0
	300	40.0	0.05856	19.0
	500	66.7	0.11064	38.0
	730	97.3	0.17634	65.4
293.2	100	13.3	0.01204	2.2
	300	40.0	0.03417	11.6
	500	66.7	0.04820	16.6
	730	97.3	0.06980	24.6

The pressures appear to be the partial pressure of fluoroethane. The compiler added the kPa pressure values. The volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 of solvent and then adjusted to 1 atm pressure. The authors give the enthalpy of solution as ΔH/kcal mol^{-1} = −7.60.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) Tetrahydrofuran.
Described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Ethanol; C_2H_6O; [64-17-5]
(2) Butanol; $C_4H_{10}O$; [71-36-3]
(2) 1,2-Ethanediol or ethylene glycol; $C_2H_4O_2$; [107-21-1]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983). J. Appl. Chem. USSR (Engl. Transl.) **56**, 2048–2051 (1983).

Variables:
T/K = 293.2
p_1 /kPa = 97.3 (730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in several alcohols at 293.2 K and a partial pressure of 97.3 kPa

Solvent	T/K	p_1 /mmHg	Mole Fraction-x_1	Volume Absorbed (V/cm^3)
Ethanol	293.2	730	0.02870	10.4
Butanol	293.2	730	0.03389	9.0
1,2-ethanediol	293.2	730	0.00222	0.1

The 730 mmHg (97.3 kPa) appears to be the partial pressure of the fluoroethane. Volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 solvent and then adjusted to 1 atm pressure.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) The alcohols.
Described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Tetrahydrofuran; C_4H_8O; [109-99-9]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983); J. Appl. Chem. USSR (Engl. Transl.) **56**, 2048–2051 (1983).

Variables:
T/K = 253.2, 273.2 and 293.2
p_1 /kPa = 13.3–97.3 (100–730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in tetrahydrofuran at 253.2 K, 373.2 K, and 293.2 K at partial pressure from 13.3 kPa to 97.3 kPa

T/K	p_1 /mmHg	p_1 /kPa	Mole Fraction x_1	Volume Absorbed (V/cm^3)
253.2	100	13.3	0.11613	16.0
	300	40.0	0.33007	60.0
	500	66.7	0.47450	110.0
	730	97.3	0.64473	221.0
273.2	100	13.3	0.03666	5.0
	300	40.0	0.08368	12.0
	500	66.7	0.19970	32.8
	730	97.3	0.28352	52.0
293.2	100	13.3	0.02083	3.0
	300	40.0	0.05999	9.0
	500	66.7	0.09613	15.0
	730	97.3	0.12960	21.0

The pressures appear to be the partial pressure of fluoroethane. The compiler added the kPa pressure values. The volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 solvent and then adjusted to 1 atm pressure. The authors give the enthalpy of solution as ΔH/kcal mol^{-1} = −6.21.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) Tetrahydrofuran.
Described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]
(2) 1,1′-Oxybis(2-methoxy)ethane or diglyme; $C_6H_{14}O_3$; [111-96-6]
(2) Acetic acid; $C_2H_4O_2$; [64-19-7]
(2) Acetic acid, ethyl ester; $C_4H_8O_2$; [141-78-6]
(2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983); J. Appl. Chem. USSR (Engl. Transl.) **56**, 2048–2051 (1983).

Variables:
T/K = 293.2
p_1 /kPa = 97.3 (730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solvent	T/K	p_1 /mmHg	Mole Fraction x_1	Volume Absorbed (V/cm^3)
1,4-Dioxane	293.2	730	0.07847	24.0
1,1′-Oxybis(2-methoxy)ethane	293.2	730	0.07274	18.0
Acetic acid	293.2	730	0.06041	27.0
Acetic acid, ethyl Ester	293.2	730	0.08214	22.0
Cyclohexanone	293.2	730	0.18312	52.0

The 730 mmHg (97.3 kPa) appears to be the partial pressure of the fluoroethane. Volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 solvent and then adjusted to 1 atm pressure.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) The oxygen containing compounds.
Described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Trichloromethane or chloroform; $CHCl_3$; [67-66-3]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983); J. Appl. Chem. USSR (Engl. Trans.) **56**, 2048–2051 (1983).

Variables:
T/K = 253.2, 273.2, and 293.2
p_1 /kPa = 13.3–97.3 (100–730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in trichloromethane at 253.2 K, 273.2 K and 293.2 K, at partial pressure from 13.3 kPa to 97.3 kPa

T/K	p_1 /mmHg	p_1 /kPa	Mole Fraction x_1	Volume Absorbed (V/cm^3)
253.2	100	13.3	0.13381	46.0
	300	40.0	0.31668	120.0
	500	66.7	0.43580	200.0
	730	97.3	0.55880	328.0
273.2	100	13.3	0.06991	21.0
	300	40.0	0.12790	41.0
	500	66.7	0.18630	64.0
	730	97.3	0.23326	85.0
293.2	100	13.3	0.00723	2.2
	300	40.0	0.03847	12.0
	500	66.7	0.07520	24.4
	730	97.3	0.09470	31.4

The compiler added the kPa pressure values. The volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 of solvent and then adjusted to 1 atm pressure. The authors give the enthalpy of solution as ΔH/kcal mol^{-1} = −6.95.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) Trichloromethane.
Both described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Tetrachloromethane; CCl_4; [56-23-5]
(2) Sulfinylbismethane or dimethylsulfoxide; C_2H_6SO; [67-68-5]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983); J. Appl. Chem. USSR (Engl. Transl.) **56**, 2048–2051 (1983).

Variables:
T/K = 293.2
p_1 /kPa = 97.3 (730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in tetrachloromethane and in dimethyl sulfoxide at 293.2 K and a partial pressure of 97.3 kPa

Solvent	T/K	p_1 /mmHg	Mole Fraction x_1	Volume Absorbed (V/cm^3)
Tetrachloromethane	293.2	730	0.12440	32.4
Sulfinylbismethane	293.2	730	0.02870	10.0

The 730 mmHg (97.3 kPa) appears to be the partial pressure of the fluoroethane. Volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 solvent and then adjusted to 1 atm pressure.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) Tetrachloromethane and Sulfinylbismethane. All described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Dimethylformamide; C_3H_7NO; [68-12-2]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983); J. Appl. Chem. USSR (Engl. Transl.) **56**, 2048–2051 (1983).

Variables:
T/K = 253.2, 273.2, and 293.2
p_1 /kPa = 13.3–97.3 (100–730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in dimethylformamide at 253.2 K, 273.2 K, and 293.2 K and partial pressures from 13.3 to 97.3 kPa

T/K	p_1 /mmHg	p_1 /kPa	Mole Fraction x_1	Volume Absorbed (V/cm^3)
253.2	100	13.3	0.10006	30.0
	300	40.0	0.19413	65.0
	500	66.7	0.27040	100.0
	730	97.3	0.32515	130.0
273.2	100	13.3	0.05212	16.0
	300	40.0	0.11544	38.0
	500	66.7	0.15645	54.0
	730	97.3	0.19383	70.0
293.2	100	13.3	0.02190	7.0
	300	40.0	0.04405	14.4
	500	66.7	0.06856	23.0
	730	97.3	0.08224	28.0

The pressures appear to be the partial pressure of fluoroethane. The compiler added the kPa pressure values. The volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 solvent and then adjusted to 1 atm pressure. The authors give the enthalpy of solution as ΔH/kcal mol^{-1} = −7.05.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) Dimethylformamide.
Both described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) 1-Methyl-2-pyrrolidinone or *N*-methylpyrrolidone; C_5H_9NO; [872-50-4]
(2) Phosphoric acid, tributyl ester; $C_{12}H_{27}O_4P$; [126-73-8]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983); J. Appl. Chem. USSR (Engl. Transl.) **56**, 2048–2051 (1983).

Variables:
T/K = 293.2
p_1 /kPa = 97.3 (730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solvent	T/K	p_1 /mmHg	Mole Fraction x_1	Volume Absorbed (V/cm^3)
1-Methyl-2-pyrrolidinone	293.2	730	0.11111	22.2
Phosphoric acid, Tributyl ester	293.2	730	0.20390	29.0

The 730 mmHg (97.3 kPa) appears to be the partial pressure of the fluoroethane. Volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 solvent and then adjusted to 1 atm pressure.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) 1-Methyl-2-pyrrolidinone and phosphoric acid, tributyl ester. Described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Quinoline; C_9H_7N; [91-22-5]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983); J. Appl. Chem. USSR (Engl. Trans.) **56**, 2048–2051 (1983).

Variables:
T/K = 253.2, 273.2, and 293.2
p_1 /kPa = 13.3–97.3 (100–730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in quinoline at 253.2 K, 273.2 K, and 293.2 K and partial pressures from 13.3 kPa to 97.3 kPa

T/K	p_1 /mmHg	p_1 /kPa	Mole Fraction x_1	Volume Absorbed (V/cm^3)
253.2	100	13.3	0.05386	10.0
	300	40.0	0.10679	21.0
	500	66.7	0.18925	41.0
	730	97.3	0.26399	63.0
273.2	100	13.3	0.01558	3.0
	300	40.0	0.04050	8.0
	500	66.7	0.08231	17.0
	730	97.3	0.11239	24.0
293.2	100	13.3	0.00973	2.0
	300	40.0	0.03327	7.0
	500	66.7	0.04686	10.0
	730	97.3	0.06696	14.6

The pressures appear to be the partial pressure of fluoroethane. The compiler added the kPa pressure values. The volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 of solvent and then adjusted to 1 atm pressure. The authors give the enthalpy of solution as ΔH/kcal mol^{-1} = −5.29.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Material:
(1) Fluoroethane.
(2) Quinoline.
Both described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1 / x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

Components:
(1) Fluoroethane; C_2H_5F; [353-36-6]
(2) Phosphoric acid, triethyl ester; $C_9H_{21}O_4P$; [78-40-0]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, Ya. N. Pirig, and T. S. Politanskaya, Zh. Prikl. Khim. **56**, 2205–2209 (1983). J. Appl. Chem. USSR (Engl. Trans.) **56**, 2048–2052 (1983).

Variables:
T/K = 253.2, 273.2, and 293.2
p_1 /kPa = 13.3–97.3 (100–730 mmHg)

Prepared By:
C. L. Young and H. L. Clever

Experimental Values

Solubility of fluoroethane in phosphonic acid, triethyl ester at 253.2 K, 273.2 K, and 293.2 K and partial pressures from 13.3 kPa to 87.3 kPa

T/K	p_1 /mmHg	p_1 /kPa	Mole Fraction x_1	Volume Absorbed (V/cm^3)
253.2	100	13.3	0.05312	14.8
	300	40.0	0.20494	68.0
	500	66.7	0.28508	105.2
	730	97.3	0.36616	152.4
273.2	100	13.3	0.01317	3.8
	300	40.0	0.07174	22.0
	500	66.7	0.10949	35.0
	730	97.3	0.17647	61.0
293.2	100	13.3	0.02083	3.0
	300	40.0	0.05999	9.0
	500	66.7	0.09613	15.0
	730	97.3	0.12690	21.0

The pressures appear to be the partial pressure of fluoroethane.
The compiler added the kPa pressure values.
The volume absorbed appears to be the volume absorbed at the T and p of the experiment by 1 cm^3 of solvent and then adjusted to 1 atm pressure.
The authors give the enthalpy of solution as ΔH/kcal mol^{-1} = −6.31.

Auxiliary Information

Method/Apparatus/Procedure:
No details in the source except static apparatus described by Braude *et al.*[1]

Source and Purity of Materials:
(1) Fluoroethane.
(2) Phosphoric acid, triethyl ester.
Both described as "chromatographically pure and dry."

Estimated Error:
δT/K = ±0.1
$\delta x_1/x_1$ = ±0.02 (estimate of compiler).

References:
[1]G. E. Braude, I. L. Leites, and N. V. Dedova, Khim. Prom-st. **1961**, 232.

3.16. Octafluoropropane

Components:
(1) Octafluoropropane; C_3F_8; [76-19-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–246 (1979).

Variables:
T/K = 278.15–288.15
p_{tot} /MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Solubility of octafluoropropane in water from 278.15 K to 288.15 K at 0.1013 MPa

t/°C	T/K	Mole Fraction $10^6 x_1$	Std. Dev. $10^6\sigma$	Ostwald Coefficient ($10^3 L$/mL mL^{-1})	Std. Dev. $10^3\sigma$	No. of Det'n.
5	278.15	1.32	0.01	1.63	0.02	3
10	283.15	0.674	0.02	0.846	0.02	6
15	288.15	0.560	0.02	0.717	0.02	4

The authors fitted their data to equations in mole fraction and the Ostwald coefficient.

$$R\ \ln(x_1/(p_1/\text{MPa})) = -20\,230.5 + 872\,216./(T/\text{K}) + 3032.55\ \ln(T/\text{K}) \qquad (\sigma = 0.70\%)$$

$$R\ \ln(L/\text{mL mL}^{-1}) = -20\,247.8 + 873\,058./(T/\text{K}) + 3037.63\ \ln(T/\text{K}) \qquad (\sigma = 1.43\%)$$

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and procedure were similar to that described by Ben-Naim and Baer[1] as modified by Wen and Hung.[2] It consists of a mercury manometer, a gas-volume measuring buret, a dissolution cell of 2.1 or 2.4 L, and a mercury reservoir. The apparatus is immersed in a water thermostat. Degassing is done with a Battino *et al.*[3] type apparatus. The cell containing the solvent is degassed, the system filled with solvent saturated gas to 1 atm total pressure. The solvent is stirred, as the gas dissolves the pressure is maintained at 1 atm until equilibrium is reached.

Source and Purity of Material:
(1) Octafluoropropane. Matheson Gas Products. Minimum purity of 99.0% was confirmed by GLC. Used as received.
(2) Water. Distilled then passed through Milli-Q system.

Estimated Error:
δT/K = ±0.005
δp/Torr = ±3
$\delta L/L$ = ±0.0064 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]W.-Y. Wen and J. H. Hung, J. Phys. Chem. **74**, 170 (1970).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 896 (1971).

Components:
(1) Octafluoropropane; C_3F_8; [76-19-7]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

Original Measurements:
K. W. Miller, Phys. Chem. **72**, 2248–2249 (1968).

Variables:
T/K = 280.15–305.45
p_1 /kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of octafluoropropane in cyclohexane from 280.15 K to 305.45 K at a partial pressure of 0.101325 MPa

Temperature (t/°C)	Temperature (T/K)	Mole Fraction 10^3x_1	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
7.0	280.15	7.215	1.53	1.57
12.8	285.95	6.786	1.43	1.50
18.7	291.85	6.407	1.34	1.43
25.0	298.15	6.071	1.26	1.38
32.2	305.35	5.711	1.17	1.31

The Bunsen and Ostwald coefficients were calculated by the compiler assuming ideal gas behavior and Henry's law is obeyed. The compiler also added the Kelvin temperatures.

Smoothed data: for use between 280.15 K and 305.35 K.

$$\ln x_1 = -26.4220 + 34.1282/(T/100\ \mathrm{K}) + 9.0360 \ln(T/100\ \mathrm{K})$$

The standard error about the regression line is 2.69×10^{-6}.

T/K	Mole Fraction-10^3x_1
283.15	6.983
288.15	6.636
293.15	6.334
298.15	6.071
303.15	5.842

Auxiliary Information

Method/Apparatus/Procedure:
The liquid is saturated with the gas at 1 atm partial pressure. The apparatus is that described by Dymond and Hildebrand[1] It uses an all-glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressure.

Source and Purity of Material:
(1) Octafluoropropane. Matheson Co. Dried before use.
(2) Cyclohexane. Matheson, Coleman and Bell Co. "Spectroquality." Used as received.

Estimated Error:
Nothing specified.

References:
[1]J. H. Dymond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Octafluoropropane; C_3F_8; [76-19-7]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:
D. F. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753–760 (1971).

Variables:
T/K = 297.21, 298.42
p/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of octafluoropropane in benzene near 298 K at a partial pressure of 0.101325 MPa

T/K	Mol Fraction 10^3x_1	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
297.21	2.431	0.611	0.665
298.42	2.445	0.614	0.671

The authors adjusted the gas solubility values to a gas partial pressure of 101.325 kPa (1 atm) by Henry's law.

The compiler calculated the Bunsen coefficients.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino, Evans, and Danforth.[2] The degassing apparatus is that described by Battino, Bogan and Wilhelm.[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred and the vacuum applied intermittently through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm. Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas and solvent vapor at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volume in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Octafluoropropane. Either Matheson Co. or Air Products and Chemicals Co. Purest grade available, minimum purity greater than 99.0 mole % (usually >99.9 mole %).
(2) Benzene. Mallinckrodt Co. Thiophene-free, analytical reagent grade. Used as received.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1/x_1$ = ±0.005

References:
[1]T. J. Morission and F. Billett, J. Chem. Soc. 2033, (1948).
[2]R. Battino, F. D. Evans, and F. D. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Octafluoropropane; C_3F_8; [76-19-7]
(2) Hexafluorobenzene; C_6F_6; [392-56-3]

Original Measurements:
D. F. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753–760 (1971).

Variables:
T/K = 297.56, 297.60
p/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of octafluoropropane in hexafluorobenzene near 298 K and at a partial pressure of 0.101325 MPa.

T/K	Mol Fraction 10^3x_1	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^{3}cm^{-3})
297.56	51.8	10.6	11.5
297.60	52.9	10.8	11.8

The authors adjusted the gas solubility values to a gas partial pressure of 101.325 kPa (1 atm) by Henry's law. The compiler calculated the Bunsen coefficients.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino, Evans, and Danforth.[2] The degassing apparatus is that described by Battino, Bogan, and Wilhelm.[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred and the vacuum applied intermittently through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm. Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas and solvent vapor at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volume in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Octafluoropropane. Either Matheson Co. or Air Products and Chemicals Co. Purest grade available, minimum purity 99.0 mole % (usually >99.9 mole %).
(2) Hexafluorobenzene. Imperial Smelting Co., Avonmouth, U.K. GC purity 99.7%, density, $\rho_{298.15}$ = 1.60596 g cm^{-3}. Purification described in Anal. Chem. **40**, 224 (1968).

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1/x_1$ = ±0.005

References:
[1]T. J. Morission and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and F. D. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

3.17. Octafluorocyclobutane

Components:
(1) Octafluorocyclobutane; c-C_4F_8; [115-18-5]
(2) Water; H_2O; [7732-18-5]

Evaluators:
Rubin Battino, Wright State University, Dayton, OH 45435
H. Lawrence Clever, Emory University, Atlanta, GA 30322
2002

Evaluation

An evaluation of the solubility of octafluorocyclobutane in water at a partial pressure of 0.101325 MPa between 278.15 K and 318.15 K.

Four papers report on the solubility of octafluorocyclobutane in water. Two of the papers are from the same laboratory. Filatkin *et al.*[1] do not report their data, but give a fitted equation, which requires knowledge of the gas critical constants. The compiler calculated solubility values at three temperatures from the author's equation. The mole fraction and Ostwald coefficient values are a factor of 10 larger than the values in the other three papers. There is doubt about these values and they are rejected for the present. Efforts to clarify the doubts about this paper are under way, but may not succeed before this goes to print.
Wen and Muccitelli[2] report six values of the solubility between 278.15 K and 303.15 K at a partial pressure of 0.10133 MPa. There are two papers from the laboratory of R. Battino: Park *et al.*[3] report one value of the solubility at 298.15 K and 010133 MPa and Scharlin and Battino[4] report four values from 288.22 K to 318.23 K and 0.10133 MPa partial pressure. The 298.15 K mole fraction solubility from the three papers is 2.20, 2.17, and 2.37×10^{-6}. The average is $(2.24\pm0.11)\times10^{-6}$. The 11 experimental values from the three papers were treated by a nonlinear regression to obtain the CGW and BK equations with three constants each. All of the 11 values fell within 2 s.d. of the equations. The results are:
CGW Equation.
$\ln x_1 = -(196.5062\pm35.7101) + (277.2389\pm50.7444)/(T/100\text{ K}) + (82.8621\pm17.1014)\ln(T/100\text{ K})$ with $r^2 = 0.9855$ and the standard error of estimate 0.0474 in $\ln x_1$. The temperature of minimum solubility is 334.6 K according to the equation.
BK Equation.
$\ln x_1 = (18.1746\pm8.6360) - (21\,580\pm5118.8360)[1/(T/\text{K})]^{-1} + (3\,663\,004\pm758\,625)[1/(T/\text{K})]^{-2}$ with $r^2 = 0.9984$ and the standard error of estimate 0.0475 in $\ln x_1$.
The CGW equation is used to construct Table 13 and Fig. 4.

References
[1]V. N. Filatkin, V. T. Plotnikov, and A. G. Alishev, Kholod. Tekh. (**No. 2**), 23–25 (1976).
[2]W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–246 (1979).
[3]T. Park, T. R. Rettich, R. Battino, D. Peterson, and E. Wilhelm, J. Chem. Eng. Data **27**, 324–326 (1982).
[4]P. Scharlin and R. Battino, Fluid Phase Equilibrium **94**, 137–147 (1994).

TABLE 13. The tentative mole fraction solubility of octafluorocyclobutane in water from 278.15 K to 318.15 K at a partial pressure of 0.10133 MPa. Also values of the Ostwald coefficient and thermodynamic changes on solution

Temperature (T/K)	Mol Fraction 10^6x_1	Ostwald Coefficient (L/cm^3 cm^{-3})	Enthalpy Change ($\Delta_{sln}H^o$/kJ mol^{-1})	Entropy Change ($\Delta_{sln}S^o$/J K^{-1} mol^{-1})	Heat Capacity Change ($\Delta_{sln}C_p{}^o$/J K^{-1} mol^{-1})
278.15	5.748	0.728	−38.92	−240.1	689
283.15	4.328	0.588	−35.43	−228.3	689
288.15	3.376	0.443	−31.99	−215.8	689
293.15	2.721	0.363	−28.54	−203.9	689
298.15	2.226	0.301	−25.10	−192.2	689
303.15	1.937	0.266	−21.65	−180.8	689
308.15	1.703	0.238	−18.21	−169.5	689
313.15	1.537	0.218	−14.76	−158.4	689
318.15	1.420	0.204	−11.32	−147.5	689

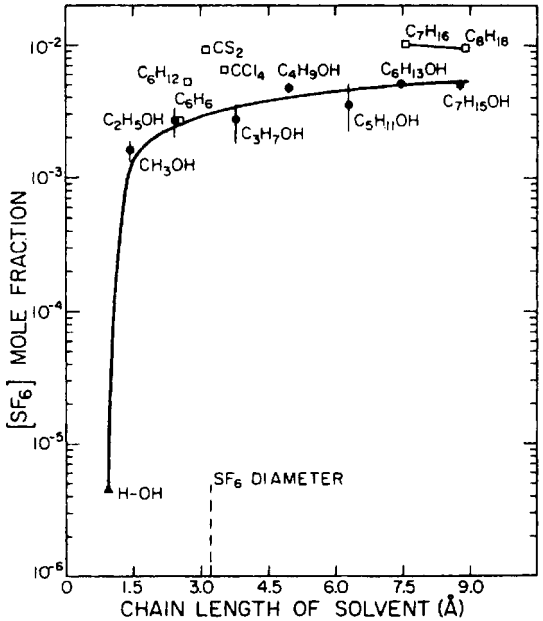

FIG. 4. The solubility of octafluorocyclobutane in water: $\ln x_1$ vs $T/(100\,\mathrm{K})$. The fitted curve and experimental points.

Components:

(1) Octfluorocyclobutane or Freon-C318; c-C_4F_8; [115-25-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. N. Filatkin, V. T. Plotnikov, and A. G. Alishev, Kholod. Tekh. (**No. 2**), 23–25 (1976).

Variables:

$T/\mathrm{K}=278.15–311.15$
$p_1/\mathrm{MPa}=0.1–0.5$

Prepared By:

Y. P. Yampolskii and H. L. Clever

Experimental Values

The data were fitted to the equation: $\ln(S/\pi)=A+B/\Theta+C/\Theta^2$, where S is the mass percent of gas in the liquid, π is the reduced pressure of the gas, $(p_1/\mathrm{MPa}/p_{1c}/\mathrm{MPa})$, and Θ is the reduced temperature of the measurement, $(T/\mathrm{K}/T_c/\mathrm{K})$.
For the Freon-C318 the equation is:

$$\ln(S/\pi[(p_1/\mathrm{MPa})/(p_{1c}/\mathrm{MPa})]=-1.1045+38\,235/[(T/\mathrm{K})/(T_c/\mathrm{K})]+0.1687/[(T/\mathrm{K})/(T_c/\mathrm{K})]^2,$$

with an average relative square deviation error of 2.6% and a maximum deviation of 5.5%.
The compiler (HLC) has calculated values of the mass percent solubility at 0.1013 MPa and three temperatures from the equation, and mole fraction and Ostwald coefficients from the mass percents at 0.1013 MPa and the temperatures of 283.15, 298.15, and 308.15 K. The *CRC Handbook*, Vol 82, 2001, gives the critical temperature as 386.4 K and the critical pressure as 2.323 MPa. The results are in the table below.

Temperature T/K	Mass percent	Mole Fraction 10^5x_1	Ostwald Coefficient $(L/\mathrm{mL\ mL^{-1}})$
283.15	0.0278	2.50	0.0322
298.15	0.0263	2.37	0.0321
308.15	0.0254	2.29	0.0320

Auxiliary Information

Method/Apparatus/Procedure:

The thermostated apparatus consisted of a saturation unit containing a Raschig ring-filled column and a hermetic pump for the re-circulation of the Freon solution and a filling tank. After equilibration is attained the dissolved Freon is desorbed by a gaseous stream of inert gas, water is absorbed by a NaX zeolite pre-column and the Freon is determined by a chromatograph equipped with thermal conductivity and flame ionization detectors.

Source and Purity of Materials:

(1) Freon-C318. Nothing specified.
(2) Water. Nothing specified.

Estimated Error:

$\delta T/\mathrm{K}=\pm0.05$
The authors stated the maximum error as 15%. See equation errors above.

Components:
(1) Octafluorocyclobutane; C_4F_8; [115-25-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W.-Y. Wen and J. A. Muccitelli, J. Solution Chem. **8**, 225–246 (1979).

Variables:
T/K = 278.15–303.15
p_{tot}/MPa = 0.1013

Prepared By:
H. L. Clever

Experimental Values

Solubility of octafluoropropane in water from 278.15 K to 288.15 K at 0.1013 MPa

t/°C	T/K	Mole Fraction $10^6 x_1$	Std. Dev. $10^6\sigma$	Ostwald Coefficient ($10^3 L$/mL mL^{-1})	Std. Dev. $10^3\sigma$	No. of Det'n
5	278.15	5.73	0.10	7.00	0.13	5
10	283.15	4.29	0.06	5.35	0.07	3
15	288.15	3.21	0.03	4.14	0.04	4
20	293.15	2.62	0.02	3.38	0.02	3
25	298.15	2.20	0.02	2.89	0.03	4
30	303.15	1.88	0.07	2.52	0.10	3

The authors fitted their data to equations in mole fraction and the Ostwald coefficient.

$$R \ln[x_1/(p_1/\text{MPa})] = -1435.93 + 67\,625.5/(T/\text{K}) + 207.671 \ln(T/\text{K}) \qquad (\sigma = 0.68\%)$$

$$R \ln(L/\text{mL mL}^{-1}) = -1580.57 + 74\,281.9/(T/\text{K}) + 231.585 \ln(T/\text{K}) \qquad (\sigma = 0.85\%)$$

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus and procedure were similar to that described by Ben-Naim and Baer[1] as modified by Wen and Hung.[2] It consists of a mercury manometer, a gas-volume measuring buret, a dissolution cell of 2.1 or 2.4 L, and a mercury reservoir. The apparatus is immersed in a water thermostat. Degassing is done with a Battino *et al.*[3] type apparatus. The cell containing the solvent is degassed, the system filled with solvent saturated gas to 1 atm total pressure. The solvent is stirred, as the gas dissolves the pressure is maintained at 1 atm until equilibrium is reached.

Source and Purity of Material:
(1) Octafluorocylcobutane. Union Carbide Co. Linde Specialty gas. Minimum purity of 99.9% was confirmed by GLC. Used as received.
(2) Water. Distilled then passed through Milli-Q system.

Estimated Error:
δT/K = ±0.005
δp/Torr = ±3
$\delta L/L$ = ±0.0064 (authors).

References:
[1]A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2]W.-Y. Wen and J. H. Hung, J. Phys. Chem. **74**, 170 (1970).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 896 (1971).

Components:
(1) Octafluorocyclobutane or Freon-C318; c-C_4F_8; [115-25-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. Park, T. R. Rettich, R. Battino, D. Peterson, and E. Wilhelm, J. Chem. Eng. Data **27**, 324–326 (1982).

Variables:
T/K = 298.15
p_1/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of CF_4 in water at 298.15 K and 101.325 kPa

T/K	No. of Detn's.	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Std. Dev.
298.15	3	0.002689	3.9

The Bunsen coefficient was measured on the modified apparatus 2. The standard deviation is given as percent standard deviation, $100\sigma/\alpha$.

Auxiliary Information

Method/Apparatus/Procedure:
Two different versions of the Scholander[1] micro-gasometric apparatus were used. They were housed in an air thermostat.
Apparatus 1 was the modified form described by Douglas[2] and by others.
Apparatus 2 was modified by the authors. The design includes a more efficient method of degassing and transferring water to the apparatus. The apparatus itself had a 4 cm^3 compensation chamber, a 10 cm^3 equilibration chamber, and an 8 cm side arm.

Source and Purity of Material:
(1) Freon-C318. Union Carbide Co. Stated to be 99.9 mol % minimum purity.
(2) Water. House distilled (reverse osmosis), passed through an ion exchange column until specific resistance was 5 $\times 10^6$ Ω cm.

Estimated Error:
δT/K = ±0.05
Solubility. See percent standard deviation above.

References:
[1]P. F. Scholander, J. Biol. Chem. **167**, 235 (1947).
[2]E. Douglas, J. Phys. Chem. **68**, 169 (1964).

Components:
(1) Octafluorocyclobutane; (Freon C 318); c-C_4F_8; [115-25-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. Scharlin and R. Battino, Fluid Phase Equilib. **94**, 137–-147 (1994).

Variables:
T/K = 288.15–318.23
p_1 /kPa = 101.325

Prepared By:
Pirketta Scharlin

Experimental Values

Ostwald coefficient and mole fraction of octafluorocyclobutane dissolved in water at 288–318 K and partial pressure of 101.325 kPa

T/K	10^2L [a,b]	10^5x_1 [c,b]	10^5x_1 [d]
288.15	–	–	0.3693
288.22	0.4673	0.3679	0.3679
298.15	–	–	0.2373
298.16	0.3119	0.2372	0.2371
308.13	0.2355	0.1734	0.1734
308.15	–	–	0.1734
318.15	–	–	0.1419
318.23	0.1984	0.1417	0.1417

[a] L = Ostwald coefficient [cm^3 cm^{-3}].
[b] Experimental value.
[c] x_1 = mole fraction of octafluorocyclobutane (corrected for nonideality).
[d] Smoothed value; calculated from the smoothing equation below $\ln x_1 = -216.105 + 306.894/(T/100\ \mathrm{K}) + 91.742 \ln(T/100\ \mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus was based on a design of Ben-Naim and Baer,[1] which had been improved by modifications described in detail in Tominaga *et al.*[2] After degassing,[3] the solvent was transferred under its own vapor pressure into the evacuated mixing chamber. The gas buret was evacuated and the system filled with the solvent-saturated gas to a total pressure of about 1 atm. The computer program controlling the apparatus read the pressure of the system, which was tracked during the measurement. When the reading was stable, the pressure was adjusted to 1 atm and the corresponding pressure transducer reading became the setpoint for pressure control. After pre-equilibration, the initial volume of solvent was determined using a precision cathetometer. The dissolution was initiated by high-speed stirring of the solvent. After the system had reached equilibrium, stirring was stopped and the final volume of solvent was recorded. Gas volume was determined by a computer counting the number of steps a stepping motor used to drive a close-fitting stainless steel or teflon piston with two O-ring seals through a Fisher and Porter precision bore tube.

Source and Purity of Material:
(1) Matheson, purity 99.99 mole %.
(2) Reverse osmosis "house-distilled."
Further purified by continuous pumping through a series of Illco-Way research model ion exchangers and through a 1.2 μm pore size Millipore filter. Degassed.

Estimated Error:
δT/K = ±0.03
$\delta p/p$ = ±0.2%
$\delta L/L$ = ±1.0%

References:
[1] A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2] T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[3] R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Octafluorocyclobutane; (Freon C 318); c-C_4F_8; [115-25-3]
(2) Water-d_2; (deuterium oxide); D_2O; [7789-20-0]

Original Measurements:
P. Scharlin and R. Battino, Fluid Phase Equilib. **94**, 137–147 (1994).

Variables:
T/K = 288.15–318.20
p_1 /kPa = 101.325

Prepared By:
Pirketta Scharlin

Experimental Values

Ostwald coefficient and mole fraction of octafluorocyclobutane dissolved in deuterium oxide at 288–318 K and partial pressure of 101.325 kPa

T/K	10^2L [a,b]	10^5x_1 [c,b]	10^5x_1 [d]
288.15	–	–	0.596
288.28	0.7398	0.585	0.592
298.15	–	–	0.352
298.17	0.4955	0.378	0.352
308.14	0.2615	0.193	0.215
308.15	–	–	0.215
318.15	–	–	0.136
318.20	0.1991	0.143	0.136

[a] L = Ostwald coefficient [cm^3 cm^{-3}].
[b] Experimental value
[c] x_1 = mole fraction of octafluorocyclobutane (corrected for nonideality).
[d] Smoothed value; calculated from the smoothing equation $\ln x_1 = -27.7119 + 45.1858/(T/100\ \mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus was based on a design of Ben-Naim and Baer,[1] which had been improved by modifications described in detail in Tominaga *et al.*[2] After degassing,[3] the solvent was transferred under its own vapor pressure into the evacuated mixing chamber. The gas buret was evacuated and the system filled with the solvent-saturated gas to a total pressure of about 1 atm. The computer program controlling the apparatus read the pressure of the system, which was tracked during the measurement. When the reading was stable, the pressure was adjusted to 1 atm and the corresponding pressure transducer reading became the setpoint for pressure control. After pre-equilibration, the initial volume of solvent was determined using a precision cathetometer. The dissolution was initiated by high-speed stirring of the solvent. After the system had reached equilibrium, stirring was stopped and the final volume of solvent was recorded. Gas volume was determined by a computer counting the number of steps a stepping motor used to drive a close-fitting stainless steel or teflon piston with two O-ring seals through a Fisher and Porter precision bore tube.

Source and Purity of Material:
(1) Matheson, purity 99.99 mole %.
(2) Isotec Inc., a Matheson USA company. Purity 99.9 mole %. Degassed.

Estimated Error:
δT/K = ±0.03
$\delta p/p$ = ±0.2%
$\delta L/L$ = ±1.0%

References:
[1] A. Ben-Naim and S. Baer, Trans. Faraday Soc. **59**, 2735 (1963).
[2] T. Tominaga, R. Battino, H. K. Gorowara, R. D. Dixon, and E. Wilhelm, J. Chem. Eng. Data **31**, 175 (1986).
[3] R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Octafluorocyclobutane; c-C_4F_8; [115-25-3]
(2) Cyclohexane; c-C_6H_{12}; [110-82-7]

Original Measurements:
K. W. Miller, J. Phys. Chem. **72**, 2248–2249 (1968).

Variables:
T/K = 280.25–307.15
p_1/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of octafluorocyclobutane in cyclohexane from 280.25 K to 307.15 K at a partial pressure of 0.101325 MPa

Temperature $(t/°C)$	Temperature (T/K)	Mole Fraction 10^3x_1	Bunsen Coefficient $[\alpha/cm^3(STP)\ cm^{-3}\ atm^{-1}]$	Ostwald Coefficient $(L/cm^3\ cm^{-3})$
7.1	280.25	29.15	6.32	6.48
8.8	281.95	28.21	6.10	6.30
16.0	289.15	24.86	5.31	5.62
25.0	298.15	21.57	4.54	4.96
34.0	307.15	19.02	3.95	4.44

The Bunsen and Ostwald coefficients were calculated by the compiler assuming ideal gas behavior and Henry's law is obeyed. The compiler also added the Kelvin temperatures.

Smoothed data for use between 280.25 K and 307.15 K:

$$\ln x_1 = -27.7896 + 41.0181/(T/100\ K) + 9.333 \ln(T/100\ K)$$

The standard error about the regression line is 1.42×10^{-5}.

T/K	Mole Fraction 10^3x_1
283.15	27.61
288.15	25.28
293.15	23.29
298.15	21.57
303.15	20.07

Auxiliary Information

Method/Apparatus/Procedure:
The liquid is saturated with the gas at 1 atm partial pressure. The apparatus is that described by Dymond and Hildebrand.[1] It uses an all-glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressure.

Source and Purity of Material:
(1) Octafluorocyclobutane. Matheson Co., Inc. Dried before use.
(2) Cyclohexane. Matheson, Coleman and Bell Co. "Spectroquality." Used as received.

Estimated Error:
Nothing specified.

References:
[1]J. H. Dymond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Octafluorocyclobutane; c-C_4F_8; [115-25-3]
(2) Benzene; C_6H_6; [71-43-2]

Original Measurements:
D. F. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753–760 (1971).

Variables:
T/K = 297.24, 297.26
p/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of octafluorocyclobutane in benzene near 297 K at a partial pressure of 0.101325 MPa

T/K	Mol Fraction 10^3x_1	Bunsen Coefficient $[\alpha/cm^3(STP)\ cm^{-3}\ atm^{-1}]$	Ostwald Coefficient $(L/cm^3\ cm^{-3})$
297.24	11.2	2.84	3.09
297.26	9.3	2.36	2.57

The authors adjusted the gas solubility values to a gas partial pressure of 101.325 kPa (1 atm) by Henry's law. The compiler calculated the Bunsen coefficients.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino, Evans, and Danforth.[2] The degassing apparatus is that described by Battino, Bogan, and Wilhelm.[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred and the vacuum applied intermittently through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas and solvent vapor at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volume in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Octafluorocyclobutane. Either Matheson Co. or Air Products and Chemicals Co. Purest grade available, minimum purity greater than 99.0 mole % (usually >99.9 mole %).
(2) Benzene. Mallinckrodt Co. Thiophene-free, analytical reagent grade. Used as received.

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1/x_1$ = ±0.005

References:
[1]T. J. Morission and F. Billett, J. Chem. Soc. 2033, (1948).
[2]R. Battino, F. D. Evans, and F. D. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Octafluorocyclobutane; c-C_4F_4; [115-25-3]
(2) Hexafluorobenzene; C_6F_6; [392-56-3]

Original Measurements:
D. F. Evans and R. Battino, J. Chem. Thermodyn. **3**, 753–760 (1971).

Variables:
T/K = 297.56, 297.60
p/kPa = 101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of octafluorocyclobutane in hexafluorobenzene near 298 K at a partial pressure of 0.101325 MPa

T/K	Mol Fraction $10^3 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})
298.15	–	–	⩾10

The solubility was larger than could be measured with the author's present equipment.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility apparatus is based on the design of Morrison and Billett[1] and the version used is described by Battino, Evans, and Danforth.[2] The degassing apparatus is that described by Battino, Bogan, and Wilhelm.[3]
Degassing. Up to 500 cm^3 of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquids is rapidly stirred and the vacuum applied intermittently through a liquid N_2 trap until the permanent gas residual pressure drops to 5 μm.
Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas and solvent vapor at a total pressure of 1 atm. The volume of gas absorbed is found by difference between the initial and final volume in the buret system. The solvent is collected in a tarred flask and weighed.

Source and Purity of Material:
(1) Octafluorocycobutane. Either Matheson Co. or Air Products and Chemicals Co. Purest grade available, minimum purity 99.0 mole % (usually >99.9 mole %).
(2) Hexafluorobenzene. Imperial Smelting Co., Avonmouth, U.K. GC purity 99.7%, density, $\rho_{298.15}$ = 1.60596 g cm^{-3}. Purification described in Anal. Chem. **40**, 224 (1968).

Estimated Error:
δT/K = ±0.03
δp/mmHg = ±0.5
$\delta x_1/x_1$ = ±0.005

References:
[1]T. J. Morission and F. Billett, J. Chem. Soc. 2033 (1948).
[2]R. Battino, F. D. Evans, and F. D. Danforth, J. Am. Oil Chem. Soc. **45**, 830 (1968).
[3]R. Battino, M. Banzhof, M. Bogan, and E. Wilhelm, Anal. Chem. **43**, 806 (1971).

Components:
(1) Octafluorocyclobutane; c-C_4F_8; [115-25-3]
(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

Original Measurements:
R. R. Hentz and W. V. Sherman, J. Phys. Chem. **72**, 2635–2641 (1968).

Variables:
T/K = ~297
P_1 /kPa not given

Prepared By:
H. L. Clever

Experimental Values

The Ostwald coefficient of c-C_4F_8 in 1,4-dioxane at about 24 °C

Temperature (T/°C)	Temperature (T/K)	Ostwald Coefficient (L/cm^3 cm^{-3})
~24	~297	1.3

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus consists of a solvent bulb, a gas and liquid mixing bulb of known volume, and a manometer.
A 100 cm^3 sample of solvent is placed in the solvent bulb. It is degassed by repeated pumping and shaking. The solvent is brought to the temperature of the solubility measurement and its vapor pressure measured.
The gas is added to the mixing bulb and its pressure measured. The gas is condensed. The degassed solvent is transferred to the mixing bulb. The mixing bulb and its contents are brought back to the temperature of the measurement and shaken vigorously to establish equilibrium. The pressure is measured, and the Ostwald coefficient is calculated from the decrease in pressure which is corrected for the solvent vapor pressure.

Source and Purity of Material:
(1) Octacyclobutane. Matheson Co., Inc. Purified by three trap to trap distillations. Degassed by pumping at −196 °C.
(2) 1,4-Dioxane. Matheson, Coleman and Bell. Spectroscopic reagent. Passed over alumina, refluxed over sodium under nitrogen atmosphere, distilled, stored under nitrogen.

Estimated Error:
$\delta L/L$ = ±0.10 (authors).

Components:
(1) Octafluorocyclobutane; C_4F_8; [115-25-3]
(2) Carbon disulfide; CS_2; [75-15-0]

Original Measurements:
R. J. Powell, J. Chem. Eng. Data **17**, 302–304 (1972).

Variables:
T/K = 273.15–303.15
p/kPa = 101.325

Prepared By:
P. L. Long and H. L. Clever

Experimental Values

T/K	Mol Fraction $10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})	Slope N ($R\Delta \log x_1)/\Delta \log T$
298.15	22.90	0.848	0.926	−4.63

The Bunsen and Ostwald coefficients were calculated by the compilers assuming ideal gas and Henry's law behavior. The author states that the solubility measurements were made over the temperature interval of about 288.15–303.15 K. Only the solubility value of 298.15 K was given in the paper. The slope, $N = R(\Delta \log x_1/\Delta \log T)$ was given. Smoothed Data: for use between 273.15 K and 303.15 K. The smoothed data was calculated by the compiler from the author's slope and solubility value at 298.15 K. The slope equation was rearranged:

$$\lg x_1 = \lg(0.002290) - (4.63/R) \lg[(T/\mathrm{K})/298.15] \text{ with } R = 1.9872 \text{ cal K}^{-1} \text{ mol}^{-1}.$$

T/K	Mol Fraction-x_1
273.15	0.002808
283.15	0.002583
293.15	0.002382
303.15	0.002203

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is the Diamond and Hildebrand[1] apparatus which uses an all glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final pressures. The solvent is degassed by freezing, pumping and followed by boiling under reduced pressure.

Source and Purity of Material:
(1) Octafluorocyclobutane. Source not given. Stated to be manufacturer's research grade, dried over $CaCl_2$ before use.
(2) Carbon disulfide. Source not given. Stated to be manufacturer's spectrochemical grade.

Estimated Error:
$\delta x_1/x_1 = \pm 0.002$
δN/cal K^{-1} mol^{-1} = ±0.1

References:
[1]J. H. Diamond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

Components:
(1) Octafluorocyclobutane; c-C_4F_8; [115-25-3]
(2) 2-Methyl pyrrolidone or N-methylpyrrolidine; C_5H_9NO; [872-50-4]

Original Measurements:
V. M. Yakovlev, I. D. Kushina, A. M. Koval'skaya, and T. I. Politanskaya, Zh. Prikl. Khim. **55**, 1325–1330 (1982); Russ. J. Appl. Chem. (Engl. Transl.) **55**, 1216–1220 (1982).

Variables:
T/K = 273.2–393.2
p_1/MPa = 0.0996

Prepared By:
H. L. Clever

Experimental Values

The absorption coefficient of c-C_4F_8 in 2-methyl pyrrolidone at temperatures from 273.15 K to 393.15 K

t/°C	T/K	Absorption Coefficient (γ/mL mL^{-1})
0	273.2	0.00
20	293.2	0.36
40	313.2	0.21
70	343.2	0.1
120	393.2	0.036

The compiler added the Kelvin temperatures. The authors used three data points to determine the coefficients of an Antoine type equation: $\ln \gamma = -12.61466 + [4666.447/(382.522 + t/°C)]$.
Henry's constant, $K_H = (f_1/\mathrm{MPa})/x_1$, and enthalpy of solution values as a function of temperature are shown in Figures. The enthalpy of solution is about −20 kcal mol^{-1} (−84 kJ mol^{-1}) at 293 K.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility coefficients were determined in an apparatus for static[1] and dynamic[2] absorption. Rapid establishment of equilibrium was achieved by either mechanical stirring or bubbling. The experiments were conducted at a pressure of 966 hPa (0.0966 MPa) over the 0 °C–120 °C temperature interval. A vapor pressure equation for the 2-methylpyrrolidone is given in the paper. The absorption coefficient *may* approximate the Ostwald coefficient.

Source and Purity of Material:
(1) Octafluorocyclobutane. Nothing specified.
(2) 2-Methylpyrrolidone. Source not given. Vacuum distilled, final water content did not exceed 0.2 mass %.

Estimated Error:
δT/K = ±0.5
$\delta\gamma/\gamma = \pm 0.05$ (compiler's estimate).

References:
[1]R. G. Makitra, G. I. Politanskaya, and F. B. Moin, Zh. Prikl Khim. **52**, 2623 (1979).
[2]I. R. Krichevskii and M. V. Koroleva, Zh. Fiz. Khim. **15**, 327 (1941).

Components:
(1) Octafluorocyclobutane; C_4F_8; [115-25-3]
(2) 1,1,2,2,3,3,4,4,4-Nonafluoro-*N*,*N*-bis(nonafluorobutyl)-1-butanamine or perfluorotributylamine; $C_{12}F_{27}N$; [311-89-7]

Original Measurements:
R. J. Powell, J. Chem. Eng. Data **17**, 302–304 (1972).

Variables:
T/K = 288.15–318.15
p/kPa = 101.325

Prepared By:
P. L. Long and H. L. Clever

Experimental Values

T/K	Mol Fraction $10^4 x_1$	Bunsen Coefficient [α/cm^3(STP) cm^{-3} atm^{-1}]	Ostwald Coefficient (L/cm^3 cm^{-3})	Slope N ($R\Delta \log x_1/\Delta \log T$)
298.15	3864.0	39.5	43.2	−17.60

The Bunsen and Ostwald coefficients were calculated by the compilers assuming ideal gas and Henry's law behavior. The author states that the solubility measurements were made over the temperature interval of about 288.15–318.15 K. Only the solubility value of 298.15 K was given in the paper. The slope, $N = R(\Delta \log x_1/\Delta \log T)$ was given.

Smoothed Data: For use between 288.15 and 318.15 K.

The smoothed data was calculated by the compiler from the author's slope and solubility value at 298.15 K. The slope equation was rearranged:

$$\lg x_1 = \lg(0.3864) - (17.60/R) \lg[(T/\mathrm{K})/298.15] \text{ with } R = 1.9872 \text{ cal K}^{-1} \text{ mol}^{-1}.$$

T/K	Mol Fraction x_1
288.15	0.5227
298.15	0.3864
308.15	0.2885
318.15	0.2174

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is the Diamond and Hildebrand[1] apparatus which uses an all glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final pressures. The solvent is degassed by freezing, pumping and followed by boiling under reduced pressure.

Source and Purity of Material:
(1) Octafluorocyclobutane. Source not given. Stated to be manufacturer's research grade, dried over $CaCl_2$ before use.
(2) Perfluorotributylamine. Minnesota Mining and Manufacturing Co. Distilled, used portion boiling between 447.85–448.64 K which gave a single GLC peak. Density at 298.15 K, $\rho = 1.880$ g cm^{-3}.

Estimated Error:
$\delta x_1/x_1 = \pm 0.002$
δN/cal K^{-1} mol^{-1} = ± 0.1

References:
[1]J. H. Diamond and J. H. Hildebrand, Ind. Eng. Chem. Fundam. **6**, 130 (1967).

3.18. Tetrafluoroethene

Components:
(1) Tetrafluoroethene; C_2F_4; [116-14-3]
(2) Water; H_2O; [7732-16-5]

Evaluators:
H. Lawrence Clever, Emory University, Atlanta, GA 30322
June 2002

Evaluation

An evaluation of the solubility of tetrafluoroethene in water at a partial pressure of 0.101325 MPa between 273.2 K and 343.2 K.

Three papers report values of the solubility of tetrafluoroethene in water. Volckhonovich *et al.*[1] report Henry's constants in several units at five degree intervals from 273.2 K to 343.2 K measured at partial pressures between 0.0200 and 0.0800 MPa; Zhang *et al.*[2] report Bunsen coefficients, mole fraction and Henry's constants at 0.10000 MPa (1 bar) at ten degree intervals from 283.15 K to 323.15 K and Sokolov and Konshin[3] report data at 298.15 K and 333.15 K. The paper of Zhang *et al.*[2] also reports a study on the salt effect of HCl and the paper of Sokolov and Konshin[3] report the effect of surface active agents on the solubility of tetrafluoroethene.

None of the papers report the mole fraction solubility at a partial pressure of 0.101325 MPa (1 atm). The evaluator has calculated the mole fraction solubility at partial pressure 0.101325 MPa from the data in each paper assuming ideal behavior and Henry's law. The results are shown in Table 14.

The evaluator classes the work of Volckhonovich *et al.*.[1] as tentative and the other two papers as doubtful. The reasoning is subjective and time may show the other papers to be equally or more reliable. The percentages show the difference between the VNZ[1] data and the values in the other papers.

Reference
I. E. Volckhonovich, E. F. Nosov, and L. B. Zorina, Zh. Fiz. Khim. **40**, 268–270 (1966); Russ. J. Phys. Chem. (Engl. Trans.) **40**, 146–148 (1966).
K. Zhang, D. Chen, G, Liu, Y. Xu, and Y. Hu, Huadong Huagong Xueyuan Xuehao (J. East China Inst. Chem. Tech) **12**(3), 343–354 (1986).
Yu. P. Sokolov and A. I. Konshin, Zh. Prikl. Khim. **63**, 678–681 (1990); J. Appl. Chem. (Engl. Transl.) **63**, 710–713 (1990).

TABLE 14. Comparison of values of tetrafluoroethene solubility in water. Various temperatures and 0.101325 MPa partial pressure

Temperature (T/K)	VNZ[1] $10^5 x_1$	ZCLXH[2] $10^5 x_1$	S & K[3] $10^5 x_1$
273.2	7.26		
278.2	5.39		
283.2	4.48	3.67 (−18%)	
288.2	3.69		
293.2	3.23	2.51 (−22%)	
298.2	2.86		1.84 (−36%)
303.2	2.59	1.90 (−27%)	
308.2	2.35		
313.2	2.15	1.45 (−33%)	
318.2	1.97		
323.2	1.85	1.18 (−36%)	
328.2	1.75		
333.2	1.69		0.81 (−52%)
338.2	1.65		
343.2	1.62		

Components:
(1) Tetrafluoroethene; C_2F_4; [116-14-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. E. Volckhonovich, E. F. Nosov, and L. B. Zorina, Zh. Fiz. Khim. **40**, 268–270 (1966); Russ. J. Phys. Chem. (Engl. Transl.) **40**, 146–148 (1966).

Variables:
T/K = 273.2–343.2
p_1 /MPa = 0.0200–0.0800

Prepared By:
H. L. Clever

Experimental Values

Temperature (t/°C)	Temperature (T/K)	Henry's Constant ($10^2 c_1$(liq)/c_1(gas))	Henry's Constant ($10^{-2} K_H$ /atm L mol^{-1})	Henry's Constant ($10^{-4} K_H$ /atm)
0.0	73.2	9.10	2.46	1.377
5.0.	278.2	6.70	3.34	1.856
10.0	283.2	5.45	4.11	2.23
15.0	88.2	4.60	4.87	2.71
20.0	93.2	4.00	5.60	3.10
25.0	98.2	3.55	6.31	3.50
30.0	03.2	3.20	7.00	3.86
35.0	08.2	2.90	7.72	4.26
40.0	13.2	2.65	8.45	4.66
45.0	18.2	2.43	9.22	5.07
50.0	23.2	2.27	9.87	5.41
55.0	328.2	2.15	10.42	5.70
60.0	33.2	2.07	10.82	5.91
65.0	38.2	2.01	11.14	6.07
70.0	43.2	1.97	11.37	6.17

The author's solubility values at five degree intervals appear to be smoothed data. They describe their values as dimensionless Henry's constants, the values appear to be Ostwald coefficients, but they are treated as Bunsen coefficients (?). They made measurements at 3–4 pressures between 150 and 600 mmHg (see Fig. 2 in paper).

The authors state that division by 22.4 converts the first column of data to a Henry's constant in the form, $K_H = (c_1$ /mol L$^{-1})/(p_1$ /atm). The compiler did the calculation and inverted the result for the second solubility data column. The compiler also calculated Henry's constant in the form $K_H = (p_1$ /atm)/x_1 in the third column and added the Kelvin temperatures.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility measurements were carried out in a glass vacuum apparatus. The water was degassed in the apparatus and a known volume of degassed water isolated. The pressure and volume of the gas was measured before contact with the water. The equilibrium pressure was measured. The dissolved gas was recovered from the saturated solution by 5–7 cycles of shaking the water and freezing out the evolved gas at liquid nitrogen temperature. The recovered gas was vaporized and its pressure measured at a known volume and temperature.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) Water. Nothing specified.

Estimated Error:
Temp.: precision ± 0.1 K.
Solubility: precision ± 3% (compiler).

Components:
(1) Tetrafluoroethene; C_2F_4; [116-14-3]
(2) Hydrogen chloride; HCl; [7647-01-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
K. Zhang, D. Chen. G. Liu, Y. Xu, and Y. Hu, Huadong Huagong Xueyuan Xuehao (J. East China Inst. Chem. Tech.) **12**(3), 343–354 (1986).

Variables:
T/K = 283.15–323.15
p_1 /MPa = 0.10000 (1.0000 bar)

Prepared By:
H. L. Clever

Experimental Values

T/K	Hydrogen Chloride (c_2 /mol L^{-1})	Bunsen Coefficient [α/cm^3(STP) cm^{-3} bar^{-1})	Mol Fraction $10^4 x_1$	Henry's Constant (K_H /MPa)	Salt Effect Parameter k_{scc}	Salt Effect Parameter k_{scx}
283.15	0.0	0.0456	0.3617	2764.5	–	–
293.15	0.0	0.0314	0.2477	4037.3	–	–
	0.4467	0.0288	0.2268	4409.3	0.084	0.086
	1.1964	0.0249	0.01977	5059.1	0.084	0.082
	2.3226	0.0212	0.1698	5916.4	0.073	0.071
	3.6073	0.0159	0.1272	7862.4	0.082	0.080
303.15	0.0	0.0236	0.1874	5336.9	–	–
	0.2294	0.0223	0.1770	5650.4	0.107	0.108
	1.3048	0.0177	0.1488	7180.0	0.096	0.077
	2.2848	0.0145	0.1155	8660.3	0.093	0.092
	3.6073	0.0104	0.0837	11951.9	0.099	0.097
	4.9213	0.0065	0.0526	19020.8	0.114	0.112
313.15	0.0	0.0180	0.1431	6988.0	–	–
	1.1741	0.0135	0.1062	9242.8	0.106	0.110
	1.8109	0.0123	0.0986	10139.6	0.091	0.089
	2.8256	0.0096	0.0735	13600.6	0.097	0.102
	3.5111	0.0067	0.0538	18587.5	0.122	0.121
	4.9210	0.0023	0.0185	54102.4	0.182	0.181
323.15	0.0	0.0145	0.1160	8621.9	–	–

Auxiliary Information

Method/Apparatus/Procedure:
A micro gas absorption apparatus modeled after that of Douglas[1] was used.

Source and Purity of Material:
(1) Tetrafluorethene. Stated to be 99.9% pure material.
(2) Hydrochloric acid. Analytical reagent grade.
(3) Water. Distilled.

Estimated Error:
δT/K = ± 0.01 (precision)
$\delta x_1 / x_1$ = ± 0.02 (compiler's estimate).

References:
[1]E. Douglas, J. Phys. Chem. **68**, 169 (1964); *ibid.* **69**, 2608 (1969).

Components:
(1) Tetrafluorethene; C_2F_4; [116-14-3]
(2) Surface active agents (SAA); See below.
(3) Water; H_2O; [7732-18-5]

Original Measurements:
Yu. P. Sokolov and A. I. Konshin, Zh. Prikl. Khim. **63**, 678–681 (1990); J. Appl. Chem. (Engl. Transl.) **63**, 710–713 (1990).

Variables:
T/K = 298.15
p_{tot} /MPa = 0.20 – 1.11

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_4 in water and in aqueous solutions of a mixture of perfluorinated surface active agents at 298.15 K and pressures between 0.20 MPa and 1.11 MPa

SAA /wt %	Pressure (p_{tot} /MPa)	C_2F_4 C (c_1 /mol L^{-1})	C_2F_4 Mol % $10^2 x_1$	Henry's Constant ($10^{-9}K_H$)	Distribution Constant ($10^2 K_d$)
0.0	0.20	0.0020	0.0036	5.5 ± 0.2	2.4 ± 0.2
	0.31	0.0030	0.0056		
	0.51	0.0050	0.0093		
	0.71	0.0070	0.013		
	0.91	0.0089	0.017		
	1.11	0.0109	0.020		
0.1	0.20	0.0023	0.0041	4.9 ± 0.3	2.8 ± 0.2
	0.31	0.0035	0.0060		
	0.51	0.0058	0.010		
	0.71	0.0082	0.014		
	0.91	0.0105	0.018		
	1.11	0.0127	0.022		
0.2	0.20	0.0021	0.0038	5.3 ± 0.2	2.6 ± 0.2
	0.31	0.0033	0.0058		
	0.51	0.0054	0.0096		
	0.71	0.0075	0.013		
	0.91	0.0096	0.017		
	1.11	0.0117	0.021		
0.3	0.20	0.0024	0.0044	4.5 ± 0.2	2.9 ± 0.2
	0.31	0.0037	0.0069		
	0.51	0.0061	0.011		
	0.71	0.0085	0.016		
	0.91	0.0109	0.020		
	1.11	0.0133	0.025		

Auxiliary Information

Method/Apparatus/Procedure:
The solubilities were measured using a 250 mL magnetically stirred reactor equipped with a pressure gage and a thermostated jacket. A volume of 100–200 mL of deaerated solvent was charged to the reactor and the gas was added. The system was equilibrated. A known volume of the saturated solution was isolated and then evaporated into a large volume. Helium carrier gas was added to bring the total pressure to 0.12 MPa. The sample was analyzed by gas chromatography.[1] Henry's constant; K_H /Pa = (p_1 /Pa)/x_1 and a distribution constant; $K_d = c_1$(liq)/c_1(gas) were calculated for water and each solution.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) SAA. A 50–50 mixture of ammonium tridecafluoroheptanoate; $NH_4C_7F_{13}O_2$; [6130-43-4] and ammonium heptadecafluorononanoate; $NH_4C_9F_{17}O_2$; [4139-60-4]. Nothing specified.
(3) Water. Nothing specified.

Estimated Error:
$\delta c_1 / c_1 = \pm 0.03 – 0.05$ (compiler's estimate).

References:
[1]Yu. P. Sokolov, A. I. Konshin, and S. V. Sokolov, Zh. Prikl. Khim. **60**, 2720 (1987).

Components:
(1) Tetrafluorethene; C_2F_4; [116-14-3]
(2) 1,1,2,3,3-Pentafluoro-3-trifluoroethenyloxy-1-propene or perfluoro propene vinyl ether or PPVE; C_5F_8O; [64080-43-9]
(3) Surface active agent (SAA); (see below)
(4) Water; H_2O; [7732-18-5]

Original Measurements:
Yu. P. Sokolov and A. I. Konshin, Zh. Prikl. Khim. **63**, 678–681 (1990); J. Appl. Chem. (Engl. Transl.) **63**, 710–713 (1990).

Variables:
T/K = 333.15
p_{tot} /MPa = 0.51 – 1.11

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_4 in a 20 wt % emulsion of 1,1,2,3,3- pentafluoro-3-trifluoro-ethenyloxy-1-propene (PPVE) in an aqueous 1.4 wt % SAA solution at 333.15 K

Temperature t/°C	Temperature T/K	Pressure (p_{tot} /MPa)	C_2F_4 C (c_1 /mol L^{-1})	C_2F_4 Mol % 10^2 x_1	Henry's Constant (K_H)	Distribution Constant (K_d)
60.0	333.15	0.51	0.00006	1.2	12.5 ± 0.5	0.95 ± 0.007
		0.71	0.00015	2.6		
		0.91	0.00023	4.1		
		1.11	0.00035	6.2		

The authors assumed all the C_2F_4 was associated with the perfluoroether (PPVE) and calculated the C_2F_4 solubility in pure PPVE. The results at several pressures were compared with interpolated values of experimental results from an earlier paper.[1] The results (see Table 2 in original paper) are:

p_{tot} /MPa	0.51	0.71	0.91	1.11	K_H /MPa
Mol % C_2F_4 Calc from 20% Emulsion	7.0	14.5	20.6	28.0	3.0 ± 0.1
Mol % C_2F_4 Interpolated[1]	9.0	15.2	21.7	28.1	3.1 ± 0.1

The authors considered the results to be the same within experimental error.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was measured using a 250 mL magnetically stirred reactor equipped with a pressure gage and a thermostated jacket. A volume of 100–200 mL of deaerated solvent was charged to the reactor and the gas was added. The system was equilibrated. A known volume of the saturated solution was isolated and then evaporated into a large volume. Helium carrier gas was added to bring the total pressure to 0.12 MPa. The sample was analyzed by gas chromatography.[1] Henry's constant; K_H /MPa = (p_1 /MPa)/x_1.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) PPVE. Nothing specified.
(3) SAA. A 50–50 mixture of ammonium tridecafluoroheptanoate; $NH_4C_7F_{13}O_2$; [6130-43-4] and ammonium heptadecafluorononanoate; $NH_4C_9F_{17}O_2$; [4139-60-4]. Nothing specified.
(4) Water. Nothing specified.

Estimated Error:
$\delta c_1 / c_1 = \pm 0.03 – 0.05$ (compiler's estimate).

References:
[1]Yu. P. Sokolov, A. I. Konshin, and S. V. Sokolov, Zh. Prikl. Khim. **60**, 2720 (1987).

Components:
(1) Tetrafluoroethene; C_2F_4; [116-14-3]
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane or Freon-113; $C_2Cl_3F_3$; [76-13-1]

Original Measurements:
R. G. Makitra, F. B. Moin, and T. I. Politanskaya, Zh. Prikl. Khim. **53**, 2553–2554 (1980); J. Appl. Chem. (Eng. transl.) **53**, 1903–1904 (1980).

Variables:
T/K = 273.15–303.15
p_1 /MPa = 0.0400–0.1360

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_4 in $C_2Cl_3F_3$ at temperatures between 273.15 K and 303.15 K and partial pressures between 0.0400 and 0.1360 MPa

Temperature		Pressure		Absorption	Mol Fraction
t/°C	T/K	(p_1/mmHg)	(p_1 /MPa)	β/mL mL^{-1}	x_1
0	273.15	300	0.0400	2.0	0.0105
		500	0.0667	5.0	0.0258
		720	0.0960	8.7	0.0446
10	283.15	720	0.0960	6.5	0.0322
20	293.15	720	0.0960	4.1	0.0199
		820	0.1093	4.5	0.0218
		920	0.1227	6.1	0.0293
		1020	0.1360	7.7	0.0367
30	303.15	720	0.0960	2.2	0.0104

The absorption coefficient appears to be: (Volume of vapor absorbed at T and p of measurement)/(Volume of solvent). The authors state Henry's law is obeyed at 0 and 20 °C. They give the enthalpy of solution as -5.73 kcal mol^{-1} (-24.0 kJ mol^{-1}).

Auxiliary Information

Method/Apparatus/Procedure:
The authors state that the solubility was determined using the usual apparatus for gas solubility determination under static conditions.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane. Nothing specified.

Estimated Error:
$\delta\alpha/\alpha = \pm 0.05$ (compiler).

Components:
(1) Tetrafluorethene; C_2F_4; [116-14-3]
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane or Freon-113; $C_2Cl_3F_3$; [76-13-1]

Original Measurements:
Yu. P. Sokolov, A. I. Konshin, and S. V. Sokolov, Zh. Prikl. Khim. **60**, 2720–2723 (1987); J. Appl. Chem. (Engl. Transl.) **60**, 2523–2523 (1987).

Variables:
T/K = 298.15–363.15
p_{tot} /MPa = 0.20–1.32

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_4 in $C_2Cl_3F_3$ at temperatures between 298.15 K and 363.15 K and pressures between 0.20 and 1.32 MPa

Temperature		Pressure	C_2F_4 Concentration	Henry's Constant	Distribution Constant
(t/°C)	(T/K)	(p_{tot} /MPa)	(c_1 /mol L^{-1})	(K_H)	(K_d)
25	298.15	0.20	0.41	3.54	6.77
		0.30	0.68		
		0.51	1.43		
		0.71	2.06		
		0.91	2.85		
		1.11	3.79		
		1.32	5.66		
50	323.15	0.20	0.22	4.11	3.88
		0.30	0.36		
		0.51	0.84		
		0.71	1.25		
		0.91	1.68		
		1.11	2.34		
		1.32	3.05		
70	343.15	0.30	0.16	4.94	2.74
		0.51	0.49		
		0.71	0.73		
		0.91	1.19		
		1.11	1.61		
		1.32	2.06		
90	363.15	0.51	0.16	7.95	1.33
		0.71	0.34		
		0.91	0.55		
		1.11	0.81		
		1.32	1.24		

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was measured using a 250 mL magnetically stirred reactor equipped with a pressure gage and a thermostated jacket. Gas and sample handling systems were attached. A volume of 100–200 mL of deaerated solvent was charged to the reactor and the gas was added. The system was equilibrated. A small liquid sample chamber was used to confine a known volume of the saturated solution. The sample was completely evaporated into a vessel of much larger volume. Helium carrier gas was added to bring the total pressure to 0.12 MPa. The sample was analyzed by gas chromatography. More details and a diagram are in the paper. Henry's constant; K_H /MPa = (p_1 /MPa)/x_1 and a distribution constant;
$K_d = [c_1(\text{liq})/\text{mol L}^{-1}]/[c_1(\text{gas})/\text{mol L}^{-1}]$ were calculated.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) 1,1,2-Trichloro-1,2,2-trifluoroethane or Freon 113 or Khladon-113. Nothing specified.

Estimated Error:
$\delta c_1/c_1 = \pm 0.03$–$0.04$ (compiler's estimate).

Note: The authors reported an enthalpy of solution of -13.6 ± 0.5 kJ mol^{-1}.

Components:
(1) Tetrafluoroethene; C_2F_4; [116-14-3]
(2) 1,2-Dibromo-1,1,2,2-tetrafluoroethane; $C_2Br_2F_4$; [124-73-2]

Original Measurements:
A. P. Krasnov, A. N. Ketov, L. K. Limonova, and N. Yu. Sudakova, Nauchn. Tr. Permsk. Politekh. Inst. (**No. 185**), 9–10 (1976).

Variables:
T/K = 283.2–313.2
p_1 /MPa = 0.1013

Prepared By:
Yu. P. Yampol'skii and H. L. Clever

Experimental Values

Solubility of tetrafluoroethene in 1,2-dibromo-1,1,2,2-tetrafluoroethane from 283.2 K to 313.2 K at a partial pressure of 0.10133 MPa

Temperature t/°C	Temperature (T/K)	Solubility (c_1 /mol L^{-1})	Ostwald Coefficient (L/cm^3 cm^{-3})
10	283.2	0.153	3.55
20	293.2	0.090	2.16
30	303.2	0.033	0.82
40	313.2	0.0107	0.275

The compiler (HLC) added the Kelvin temperatures and calculated the Ostwald coefficients assuming ideal gas behavior.

Auxiliary Information

Method/Apparatus/Procedure:
A static volumetric method was used. The thermostated absorber was magnetically stirred.
Rates of solution were also studied in this work.

Source and Purity of Material:
(1) Tetrafluoroethene. Stated to be 99.9 mole %.
(2) 1,2-Dibromo-1,1,2,2-tetrafluoroethane. Stated to be 99.92 mole %.

Estimated Error:
Nothing specified.

Components:
(1) Tetrafluoroethene; C_2F_4; [116-14-3]
(2) 1,2-Dibromo-1,1,2,2-tetrafluoroethane; $C_2Br_2F_4$; [124-73-2]

Original Measurements:
A. P. Krasnov, L. K. Limonova, O. N. Ermolaeva, and A. N. Ketov, Dep. Document VINITI **1975** 3539–3575; Zh. Fiz. Khim. **50**(3), 811 (1975).

Variables:
T/K = 273.2–303.2
p_1 /MPa = 0.0253–0.1013

Prepared By:
Yu. P. Yampol'skii and H. L. Clever

Experimental Values

Solubility of tetrafluoroethene in 1,2-dibromo-1,1,2,2-tetrafluoroethane from 273.2 K to 303.2 K at a partial pressure of 0.1013 MPa

Temperature t/°C	Temperature (T/K)	Solubility (c_1 /mol L^{-1})	Ostwald Coefficient (L/cm^3 cm^{-3})
0	273.2	0.303	6.79
10	283.2	0.182	4.23
20	293.2	0.097	2.33
30	303.2	0.050	1.24

The concentration values at 0.1013 MPa were taken from a graph by the compiler (YPY).
The compiler (HLC) added the Kelvin temperatures and calculated the Ostwald coefficients assuming ideal gas behavior.

Vant Hoff Parameters are given:
ΔH/kJ mol^{-1} = 42.7
ΔS/J K^{-1} mol^{-1} = 165 ± 0.04

Auxiliary Information

Method/Apparatus/Procedure:
A flow type apparatus[1] was used. It was equipped with a chromatographic detector to measure the composition of the saturated solution. The partial pressure of the solute gas was adjusted from 0.25 to 1 atm (0.0253–0.1013 MPa) by using a C_2F_4 + Ar gas mixture. Results were in graphs.

Source and Purity of Material:
(1) Tetrafluoroethene. Purity reported to be 99.9%.
(2) 1,2-Dibromo-1,1,2,2-tetrafluoroethane. Purity reported to be 99.6%.

Estimated Error:
Nothing specified.

References:
[1]S. M. Velichko, Ya. A. Treger, and R. M. Flid, Zh. Fiz. Khim. **47**, 2891 (1973).

Components:
(1) Tetrafluoroethene; C_2F_4; [116-14-3]
(2) Octafuorocyclobutane; C_4F_8; [115-25-3]

Original Measurements:
V. V. Tishina, L. M. Borovnev, N. S. Shirokova, L. G. Kochkina, and N. N. Loginova, Zh. Prikl. Khim. **62**, 416–418 (1989); Russ. J. Appl. Chem. (Engl. Transl.) **62**, 373–376 (1989).

Variables:
T/K = 283–333
p/MPa = 0.2–2.0

Prepared By:
H. L. Clever

Experimental Values

Temperature (T/K)	Henry's Constant [$K_H = (c_{1\,\mathrm{liq}})/(c_{1\,\mathrm{gas}})$]	Number of Points	Correlation Coefficient r_{xy}
283	11.8 ± 2.6	6	0.962
293	10.7 ± 2.2	6	0.976
303	10.2 ± 2.0	8	0.982
313	9.7 ± 2.1	7	0.976
323	8.7 ± 2.0	6	0.968
333	8.2 ± 1.4	6	0.982

The values given by the authors as Henry's constants are slopes of graphs of the equilibrium concentration of C_2F_4 in the liquid phase vs the equilibrium concentration of C_2F_4 in the vapor phase at 4–6 different pressures at a given temperature. The experimental data are shown in the paper on graphs of the inverse slope. Only the slopes by the method of least squares are tabulated. The pressure range is the total pressure. The solvent vapor pressure was known and it was subtracted from the total pressure to obtain the C_2F_4 partial pressure. The values appear to be Ostwald coefficients.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium between gas and solvent was established in a special 1.7 L high pressure autoclave equipped with a propeller stirrer (1400 rpm). A 500 g sample was loaded into the autoclave. The solvent vapor pressure was determined. The C_2F_4 gas was added from a 2.06 L buffer volume in increments of 0.2–0.3 MPa. After each addition, equilibrium was established and the total pressure measured. The C_2F_4 solubility was determined by the difference in total pressure and solvent vapor pressure by a method described earlier.[1] The compressibility of the C_2F_4 at the p and T of the experiment was taken into account.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) Octfluorocyclobutane. Nothing specified.

Estimated Error:
δT/K not specified.
δp/MPa = ± 0.01
$\delta K_H/K_H$ = ± 0.15 (compiler's estimate).

References:
[1] I. E. Volokhonovich, E. F. Nosov, and L. B. Zorina, Zh. Fiz. Khim. **40**, 268–270 (1966).

Components:
(1) Tetrafluorethene; C_2F_4; [116-14-3]
(2) Dodecafluorohexene or IPH (isomer mixture); C_6F_{12}; [86498-67-1]

Original Measurements:
Yu. P. Sokolov and A. I. Konshin, Zh. Prikl. Khim. **62**, 1395–1398 (1989); J. Appl. Chem. (Eng. transl.) **62**, 1310–1312 (1989).

Variables:
T/K = 298.15–353.15
p_{tot}/MPa = 0.20–1.32

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_4 in C_6F_{12} at temperatures between 298.15 K and 353.15 K and pressures between 0.20 and 1.32 MPa

Temperature t/°C	Temperature (T/K)	Pressure (p_{tot}/MPa)	C_2F_4 C (c_1/mol L^{-1})	Henry's Constant (K_H)	Distribution Constant (K_d)
25	298.15	0.31	0.78	2.63	7.63
		0.51	1.39		
		0.71	1.93		
		0.91	2.58		
		1.11	3.27		
		1.32	4.46		
50	323.15	0.20	0.15	3.10	6.40
		0.31	0.28		
		0.51	0.58		
		0.71	1.07		
		0.91	1.71		
		1.11	2.29		
70	343.15	0.31	0.12	3.91	5.02
		0.51	0.45		
		0.71	0.79		
		0.91	1.19		
		1.11	1.50		
		1.32	1.89		
80	353.15	0.51	0.25	4.34	4.37
		0.71	0.57		
		0.91	0.88		
		1.11	1.14		
		1.32	1.47		

Auxiliary Information

Method/Apparatus/Procedure:
The solubility were measured using a 250 mL magnetically stirred reactor equipped with a pressure gage and a thermostated jacket. Gas and sample handling systems were attached. A volume of 100–200 mL of deaerated solvent was charged to the reactor and the gas was added. The system was equilibrated. A small liquid sample chamber was used to confine a known volume of the saturated solution. The sample was completely evaporated into a vessel of much larger volume. Helium carrier gas was added to bring the total pressure to 0.12 MPa. The sample was analyzed by gas chromatography.[1]
Henry's constant; K_H/MPa = (p_1/MPa)/x_1 and a distribution constant; $K_d = c_1(\mathrm{liq})/c_1(\mathrm{gas})$ were calculated.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) The authors used the names perfluorohexene isomers mixture or IPH. Nothing specified.

Estimated Error:
$\delta c_1/c_1$ = ± 0.03 (compiler's estimate).

References:
[1] Yu. P. Sokolov, A. I. Konshin, and S. V. Sokolov, Zh. Prikl. Khim. **60**, 2720 (1987).

Note: The authors reported an enthalpy of solution of −8.5 ± 0.3 kJ mol^{-1}.

Components:
(1) Tetrafluorethene; C_2F_4; [116-14-3]
(2) Octadecafluorononene or IPN; C_9F_{18}; [79772-66-0]

Original Measurements:
Yu. P. Sokolov and A. I. Konshin, Zh. Prikl. Khim. **62**, 1395–1398 (1989); J. Appl. Chem. (Eng. transl.) **62**, 1310–1312 (1989).

Variables:
T/K = 298.15–353.15
p_{tot}/MPa = 0.20–1.11

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_4 in C_5F_8O at temperatures between 298.15 K and 363.15 K and pressures between 0.20 and 1.11 MPa

Temperature (t/°C)	Temperature (T/K)	Pressure (p_{tot}/MPa)	C_2F_4 C (c_1/mol L^{-1})	Henry's Constant (K_H)	Distribution Constant (K_d)
25	298.15	0.20	0.20		7.41
		0.31	0.71		
		0.51	1.42	No	
		0.71	1.88	Values	
		0.91	2.49	Given	
		1.11	3.13		
50	323.15	0.20	0.14		6.33
		0.31	0.30		
		0.51	0.56		
		0.71	1.10		
		0.91	1.77		
		1.11	2.30		
70	343.15	0.20	0.10		5.10
		0.31	0.41		
		0.51	0.44		
		0.71	0.83		
		0.91	1.22		
80	353.15	0.20	0.06		4.21
		0.31	0.11		
		0.51	0.20		
		0.71	0.50		
		0.91	0.81		
		1.11	1.01		

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was measured using a 250 mL magnetically stirred reactor equipped with a pressure gage and a thermostated jacket. Gas and sample handling systems were attached. A volume of 100–200 mL of deaerated solvent was charged to the reactor and the gas was added. The system was equilibrated. A small liquid sample chamber was used to confine a known volume of the saturated solution. The sample was completely evaporated into a vessel of much larger volume. Helium carrier gas was added to bring the total pressure to 0.12 MPa. The sample was analyzed by gas chromatography.[1]
The distribution constant;
$K_d = [c_1(\text{liq})/\text{mol L}^{-1}]/[c_1(\text{gas})/\text{mol L}^{-1}]$ was calculated.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) The authors used the names perfluorononene isomers mixture or IPH. Nothing specified.

Estimated Error:
$\delta c_1/c_1 = \pm 0.03$–$0.05$ (compiler's estimate).

References:
[1]Yu. P. Sokolov, A. I. Konshin, and S. V. Sokolov, Zh. Prikl. Khim. **60**, 2720 (1987).

Note: The authors reported an enthalpy of solution of -8.3 ± 0.3 kJ mol^{-1}.

Components:
(1) Tetrafluorethene; C_2F_4; [116-14-3]
(2) 1,1,2,3,3-Pentafluoro-3-trifluoroethenyloxy-1-propene or perfluoro propene vinyl ether; C_5F_8O; [64080-43-9]

Original Measurements:
Yu. P. Sokolov and A. I. Konshin, Zh. Prikl. Khim. **63**, 678–681 (1990); J. Appl. Chem. (Engl. Transl.) **63**, 710–713 (1990).

Variables:
T/K = 298.15–363.15
p_{tot}/MPa = 0.20–1.11

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_4 in C_5F_8O at temperatures between 298.15 K and 363.15 K and pressures between 0.20 and 1.11 MPa

Temperature (t/°C)	Temperature (T/K)	Pressure (p_{tot}/MPa)	C_2F_4 C (c_1/mol L^{-1})	Henry's Constant (K_H)	Distribution Constant (K_d)
25	298.15	0.20	0.41	2.10	8.65
		0.31	0.80		
		0.51	1.32		
		0.71	1.74		
		0.91	2.90		
		1.11	3.30		
50	323.15	0.31	0.32	2.81	6.95
		0.51	0.78		
		0.71	1.32		
		0.91	1.90		
		1.11	2.35		
70	343.15	0.51	0.36	3.44	5.24
		0.71	0.74		
		0.91	1.03		
		1.11	1.49		
90	363.15	0.51	0.01	4.19	3.39
		0.71	0.25		
		0.91	0.49		
		1.11	0.68		

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was measured using a 250 mL magnetically stirred reactor equipped with a pressure gage and a thermostated jacket. Gas and sample handling systems were attached. A volume of 100–200 mL of deaerated solvent was charged to the reactor and the gas was added. The system was equilibrated. A small liquid sample chamber was used to confine a known volume of the saturated solution. The sample was completely evaporated into a vessel of much larger volume. Helium carrier gas was added to bring the total pressure to 0.12 MPa. The sample was analyzed by gas chromatography.[1]
Henry's constant; $K_H/\text{MPa} = (p_1/M\text{Pa})/x_1$ and a distribution constant; $K_d = c_1(\text{liq})/c_1(\text{gas})$ were calculated.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) The authors used the names perfluoro propylene vinyl ether or PPVE. Nothing specified.

Estimated Error:
$\delta c_1/c_1 = \pm 0.03$ (compiler's estimate).

References:
[1]Yu. P. Sokolov, A. I. Konshin, and S. V. Sokolov, Zh. Prikl. Khim. **60**, 2720 (1987).

Note: The authors reported the enthalpy of solution as -9.5 ± 0.2 kJ mol^{-1}.

Components:
(1) Tetrafluoroethene; C_2F_4; [116-14-3]
(2) 1,1,1,2,2,3,3,-Heptafluoro-3-(trifluoroethenyl) oxy-propane or prefluoropropylvinyl ether; $C_5F_{10}O$; [1623-05-8]

Original Measurements:
V. V. Tishina, L. M. Borovnev, N. S. Shirokova, L. G. Kochkina, and N. N. Loginova, Zh. Prikl. Khim. **62**, 416–418 (1989); Russ. J. Appl. Chem. (Eng. transl.) **62**, 373–376 (1989).

Variables:
T/K = 283–333
p/MPa = 0.2–2.0

Prepared By:
H. L. Clever

Experimental Values

Temperature (T/K)	Henry's Constant [$K_H = (c_{1liq})/(c_{1gas})$]	Number of Points	Correlation Coefficient r_{xy}
283	15.5 ± 2.2	5	0.996
293	11.8 ± 1.5	6	0.997
303	9.8 ± 1.2	6	0.997
313	8.4 ± 0.9	6	0.998
323	7.5 ± 0.8	6	0.997
333	6.6 ± 0.8	4	0.996

The values given by the authors as Henry's constants are slopes of graphs of the equilibrium concentration of C_2F_4 in the liquid phase vs the equilibrium concentration of C_2F_4 in the vapor phase at 4–6 different pressures at a given temperature. The experimental data are shown in the paper on graphs of the inverse slope. Only the slopes by the method of least squares are tabulated. The pressure range is the total pressure. The solvent vapor pressure was known and it was subtracted from the total pressure to obtain the C_2F_4 partial pressure. The values appear to be Ostwald coefficients.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium between gas and solvent was established in a special 1.7 L high pressure autoclave equipped with a propeller stirrer (1400 rpm). A 500 g sample was loaded into the autoclave. The solvent vapor pressure was determined. The C_2F_4 gas was added from a 2.06 L buffer volume in increments of 0.2–0.3 MPa. After each addition, equilibrium was established and the total pressure measured. The C_2F_4 solubility was determined by the difference in total pressure and solvent vapor pressure by a method described earlier.[1] The compressibility of the C_2F_4 at the p and T of the experiment was taken into account.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) Perfluoropropylvinylether. Nothing specified.

Estimated Error:
δT/K not specified.
δp/MPa = ± 0.01
$\delta K_H/K_H$ = ± 0.10 (compiler'sestimate).

References:
[1]I. E. Volokhonovich, E. F. Nosov, and L. B. Zorina, Zh. Fiz. Khim. **40**, 268–270 (1966).

Components:
(1) Tetrafluorethene; C_2F_4; [116-14-3]
(2) 1,1,2,2,3,3,4,4,5,5,6,6-Dodecafluoro-1,6-*bis*(trifluoromethoxy-hexane); $C_8F_{18}O_2$; [647-40-5]

Original Measurements:
Yu. P. Sokolov and A. I. Konshin, Zh. Prikl. Khim. **62**, 1395–1398 (1989); J. Appl. Chem. (Engl. Transl.) **62**, 1310–1312 (1989).

Variables:
T/K = 293.15–333.15
p_{tot}/MPa = 0.20–0.91

Prepared By:
H. L. Clever

Experimental Values

Solubility of C_2F_4 in $C_8F_{18}O_2$ at temperatures between 293.15 K and 333.15 K and pressures between 0.20 and 0.91 MPa

Temperature (t/°C)	(T/K)	Pressure (p_{tot}/MPa)	C_2F_4 C c_1/mol L^{-}	Henry's Constant (K_H)	Distribution Constant (K_d)
20	293.15	0.20	0.55	2.37	6.00
		0.31	0.70		
		0.51	1.21		
		0.71	1.68		
		0.91	1.96		
40	313.15	0.20	0.25	3.16	4.34
		0.31	0.41		
		0.51	0.66		
		0.71	1.07		
		0.91	1.43		
60	333.15	0.20	0.12	5.48	2.38
		0.31	0.23		
		0.51	0.28		
		0.71	0.33		
		0.91	0.74		

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was measured using a 250 mL magnetically stirred reactor equipped with a pressure gage and a thermostated jacket. Gas and sample handling systems were attached. A volume of 100–200 mL of deaerated solvent was charged to the reactor and the gas was added. The system was equilibrated. A small liquid sample chamber was used to confine a known volume of the saturated solution. The sample was completely evaporated into a vessel of much larger volume. Helium carrier gas was added to bring the total pressure to 0.12 MPa. The sample was analyzed by gas chromatography.[1]
The distribution constant;
$K_d = [c_1(\text{liq})/\text{mol L}^{-1}]/[c_1(\text{gas})/\text{mol L}^{-1}]$ and Henry's constant K_H/MPa = $(p_1$/MPa$)/x_1$ were calculated.

Source and Purity of Material:
(1) Tetrafluoroethene. Nothing specified.
(2) The authors used the names perfluorohexene isomers mixture or IPH. Nothing specified.

Estimated Error:
$\delta c_1/c_1$ = ± 0.03–0.04 (compiler's estimate).

References:
[1]Yu. P. Sokolov, A. I. Konshin, and S. V. Sokolov, Zh. Prikl. Khim. **60**, 2720 (1987).

Note: The authors reported an enthalpy of solution of − 16.8 ± 0.9 kJ mol^{-1}.

3.19. 1,1-Difluoroethene

Components:
(1) 1,1-Difluoroethene or vinylidine fluoride; $C_2H_2F_2$; [75-38-7]
(2) Water; H_2O; [7732-18-5]
(2) Rat blood and liver, muscle and fat tissues

Original Measurements:
M. E. Medinsky, W. E. Bechtold, L. S. Birnbaum, D. M. Chico, R. F. Gerlach, and R. F. Henderson, Fundam. Appl. Toxicol. **11**, 250–260 (1988).

Variables:
T/K = 310.2
p_1 /kPa = 1.3 (Compiler's estimate).

Prepared By:
H. L. Clever

Experimental Values

Solvent	Temperature (t/°C)	Temperature (T/K)	Partition Coefficient $[P_1 = (c_{1(liq)})/(c_{1(gas)})]$	Confidence Interval 95%
Water	37.0	310.2	0.07±0.08	−0.08–0.23
Rat blood	37.0	310.2	0.18±0.05	0.08–0.28
Rat liver tissue	37.0	310.2	0.89±0.65	−0.73–2.33
Rat muscle tissue	37.0	310.2	0.29±0.22	−0.21–0.79
Rat fat tissue	37.0	310.2	1.0±0.2	0.53–1.47

The authors do not state the partial pressure of 1,1-difluoroethene used in the tissue/CF_2CH_2 (air) partition coefficient measurements. Their animal experiments were done at 13 000 ppm in air or argon, which would correspond to a 10 mmHg (1320 Pa) maximum partial pressure of CF_2CH_2 in air or argon.

Table 2 of the original paper gives liver/blood, tissue/blood and fat/blood partition coefficients calculated from the measured values above.

Auxiliary Information

Method/Apparatus/Procedure:
The vial equilibration method of Sato and Nakajima[1] was used. No further details were presented in the paper. The method requires vials of identical volume. In one is the sample, in both is the same amount of solute vapor. Analysis of the head-space is made by GC.
The liver, muscle, and fat samples from male F344/N rats were homogenized in 2 volumes of deionized water for each volume of tissue. The tissue/air partition coefficients were corrected for the CF_2CH_2 dissolved in the water.

Source and Purity of Material:
(1) 1,1-Difluoroethene. Pflatz and Bauer, Waterbury, CT. Certified to be better than 99% pure. The authors state the literature normal boiling point is −82 °C.
(2) Water. Deionized.
(2) Rat blood and tissues. See comments in procedure.

Estimated Error:
Temperature: Nothing specified.
Solubility: See standard errors in table above.

References:
[1]A. Sato and T. Nakajima, Br. J. Ind. Med. **36**, 231 (1979).

Components:
(1) 1,1-Difluoroethene; $C_2H_2F_2$; [1320-41-8]
(2) Ethanol; C_2H_6O; [64-17-5]
(2) Trichloromethane or chloroform; $CHCl_3$; [67-66-3]

Original Measurements:
F. Swarts, Bull. Cl. Sci., Acad. R. Belg. **7**, 383–414 (1901); See Abstr. J. Chem. Soc. **82**, 129–130 (1902).

Variables:
T/K = 293

Prepared By:
H. L. Clever

Experimental Values

Some solubilities of 1,1-difluoroethene in ethanol and chloroform at 20 °C and ambient pressure (data may be of historical interest).

Ethanol; CH_3CH_2OH; [64-17-5]
Ethanol absorbs 1.5 times its own volume of 1,1-difluoroethene gas at 20 °C.

Chloroform; $CHCl_3$; [67-66-3]
Chloroform absorbs 1.5 times its own volume of 1,1-difluoroethene gas at 20 °C.

Both 1,1-difluoroethene and difluorodiethyl ether are formed on heating 1,1-difluoro-2-bromoethane with alcoholic KOH. The CF_2CH_2 is separated and purified. It has a gas density of 2.21.

Components:
(1) 1,1-Difluoro-2-methoxy-ethane; $CHF_2CH_2OCH_3$; [461-57-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. Swarts, Bull. CL. Sci. Acad. R. Belg. **7**, 383–414 (1901); See also J. Chem. Soc. **82**, 129–130 (1902).

Variables:
T/K = 293

Prepared By:
H. L. Clever

Experimental Values

Water; H_2O; [7732-18-5] 100 volumes of water dissolves 5 volumes of 1,1-difluoro-2-methoxyethane vapor.
The 1,1-difluoro-2-methoxyethane boils at 47 °C.

3.20. Fluoroethene

Components:
(1) Fluoroethene; C_2H_3F; [75-02-5]
(2) Water; H_2O; [7732-18-5]
(2) Ethanol; C_2H_6O; [64-17-5]
(2) Acetone; C_2H_6O; [67-64-1]

Original Measurements:
F. Swarts, Bull. Cl. Sci., Acad. R. Belg. **7**, 383–414 (1901); See Abstr. J. Chem. Soc. **82**, 129–130 (1902).

Variables:
T/K = 293

Prepared By:
H. L. Clever

Experimental Values

(K_d) Solubility of fluoroethene in water, ethanol and acetone at 20 °C and ambient pressure (data may be of historical interest).

Water; H_2O; [7732-18-5]-	Fluoroethene is insoluble in water at 20 °C.
Ethanol; CH_3CH_2OH; [64-17-5]-2-	Ethanol absorbs four times its own volume of fluoroethene gas at 20 °C
Propanone or Acetone; CH_3COCH_3 ; [67-64-1]-	Acetone absorbs 5.5 times its own volume of fluoroethene gas at 20 °C.

Auxiliary Information

Method/Apparatus/Procedure:
Nothing specified.

Source and Purity of Material:
(1) Fluoroethene. Prepared from CHF_2CH_2Br by reduction with zinc in NaOH solution. A colorless odorless gas that did not solidify at liquid air temperature.
(2) Solvents. Nothing specified.

Estimated Error:
Compiler's estimate 20%.

Components:
(1) Fluoroethene or vinyl fluoride; C_2H_3F; [75-02-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, and G. P. Kostyk, Dep. Doc. **1982** VINITI 1733-82.

Variables:
T/K = 283.2–303.2
p_1 /MPa = 0.0133–0.0973

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

The mole fraction solubility of fluoroethene in water at 10 °C, 20 °C, and 30 °C, and pressures of 100 mmHg, 300 mmHg, 500 mmHg, and 730 mmHg.

Temperature		Pressure		Mol Fraction
(T/°C)	(T/K)	(p_1 /mmHg)	(p_1 /MPA)	$10^4 x_1$
10	283.2	100	0.0133	0.620
		300	0.0400	1.938
		500	0.0667	3.255
		730	0.0873	4.645
20	293.2	100	0.0133	0.374
		300	0.0400	1.273
		500	0.0667	2.246
		730	0.0973	2.994
30	303.2	100	0.0133	0.217
		300	0.0400	0.724
		500	0.0667	1.086
		730	0.0973	1.448

The compiler (HLC) added the Kelvin temperatures and the MPa pressures. The authors give a heat of absorption of 8.95 kcal mol^{-1} (37.4 kJ mol^{-1}).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is described in another paper.[1]
The authors state Henry's law is obeyed.

Source and Purity of Material:
(1) Fluoroethene. Source not given. Stated to be chromatographically pure.
(2) Water. Distilled.

Estimated Error:
Nothing specified.

References:
[1]G. E. Baude, I. L. Leites, and I. R. Dedova, Khim. Prom. **No. 4**, 232 (1961).

Components:
(1) Fluoroethene or vinyl fluoride; C_2H_3F; [75-02-5]
(2) 2-Propanone or acetone; C_3H_6O; [67-64-1]
(2) Ethyl acetate; $C_4H_8O_2$; [141-78-5]

Original Measurements:
T. S. Sirlibaev, E. F. Narkhodzhaev, A. A. Yul'chibaev, and Kh. U. Usamnov, Nauch. Tr. Tashkent Un-r. **No. 462**, 103–105 (1974).

Variables:
T/K = 283.2–313.2
p_1 /MPa = 0.81–1.22

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

Solubility of fluoroethene in acetone and in ethyl acetate at temperatures between 10 °C and 40 °C at pressures of 8 atm and 12 atm (0.81 MPa and 1.22 MPa)

Temperature		Pressure		Solubility
(T/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	cm^3 (STP) g^{-1}
Acetone				
10		8	0.81	280
	283.2	12	1.22	528
15		8	0.81	239
	288.2	12	1.22	454
20		8	0.81	206
	293.2	12	1.22	371
30		8	0.81	148
	303.2	12	1.22	239
40		8	0.81	116
	313.2	12	1.22	182
Ethyl acetate				
10		8	0.81	289
	283.2	12	1.22	594
15		8	0.81	248
	288.2	12	1.22	528
20		8	0.81	190
	293.2	12	1.22	363
30		8	0.81	99
	303.2	12	1.22	223
40		8	0.81	74
	313.2	12	1.22	165

The compiler (YPY) took the values from small graphs in the original paper.
The compiler (HLC) added the Kelvin temperatures and the MPa pressures.

Auxiliary Information

Method/Apparatus/Procedure:
The volumetric apparatus is described in another paper.[1]
The systems appear to be quite non-ideal. The simple Henry's law is only approached at the higher temperatures.

Source and Purity of Material:
(1) Fluoroethene. Nothing specified.
(2) Acetone. Nothing specified.
(2) Ethyl acetate. Nothing specified.

Estimated Error:
Nothing specified.

References:
[1]E. R. Shenderei, Ya. D. Zel'venskii, and F. P. Ivanovskii, Khim. Prom. **No. 5**, 370 (1960).

Components:
(1) Fluoroethene or vinyl fluoride; C_2H_3F; [75-02-5]
(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

Original Measurements:
E. F. Narkhodzhaev, T. S. Sirlibaev, A. A. Yul'chibaev, and Kh. U. Usamnov, Uxb. Khim. Zh. **19**(3), 19–20 (1975).

Variables:
T/K = 285.2–303.2
p_1 /MPa = 0.0153–0.0975

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

The mole fraction solubility of fluoroethene in 1,4-dioxane at 12 °C, 20 °C, and 30 °C and pressures between 115 mmHg and 734 mmHg

Temperature		Pressure		Mol Fraction
(T/°C)	(T/K)	(p_1 /mmHg)	(p_1 /MPa)	x_1
12	285.2	127	0.0169	0.007
		230	0.0307	0.013
		350	0.0467	0.020
		426	0.0568	0.030
		563	0.0751	0.033
		650	0.0867	0.037
20	293.2	115	0.0153	0.004
		238	0.0317	0.010
		352	0.0469	0.017
		534	0.0712	0.027
		641	0.0855	0.033
		716	0.0955	0.037
30	303.2	143	0.0191	0.004
		281	0.0375	0.010
		378	0.0504	0.015
		507	0.0676	0.021
		651	0.0868	0.027
		734	0.0979	0.031

The compiler (HLC) added the Kelvin temperatures and the MPa pressures. The authors conclude that Henry's law is obeyed.

Auxiliary Information

Method/Apparatus/Procedure:
Static method. The apparatus is described in another paper.[1]

Source and Purity of Material:
(1) Fluoroethene. Nothing specified.
(2) 1,4-Dioxane. Nothing specified.

Estimated Error:
Nothing specified.

References:
[1]G. E. Baude, and S. F. Shahova, Khim. Prom. **No. 3**, 177 (1961).

Components:
(1) Fluoroethene or vinyl fluoride; C_2H_3F; [75-02-5]
(2) 2-(2-Furanyl)-1,3-dioxolane; $C_7H_8O_3$; [1708-41-4]

Original Measurements:
F. B. Moin, T. I. Politanskaya, E. I. Zaitsev, A. M. Zaliznyi, and R. G. Makitra, Dep. Document **1975** VINITI 2396-75; Zh. Fiz. Khim. **47**(11), 3016 (1975).

Variables:
T/K = 243.2–338.2
p_1 /MPa = 0.0133–0.0967

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

The mole fraction solubility of fluoroethene in 2-(2-furanyl)-1,3-dioxolane between −20 °C and 65 °C and pressures between 100 mmHg and 725 mmHg

Temperature		Pressure		Mol Fraction
(T/°C)	(T/K)	(p_1 /mmHg)	(p_1 /MPa)	10^2x_1
−20	253.2	100	0.0133	0.075
		300	0.0400	0.264
		500	0.0667	0.435
		725	0.0967	0.640
0	273.2	100	0.0133	0.064
		300	0.0400	0.185
		500	0.0667	0.329
		725	0.0967	0.435
20	293.2	100	0.0133	0.053
		300	0.0400	0.148
		500	0.0667	0.254
		725	0.0967	0.329
35	308.2	100	0.0133	0.032
		300	0.0400	0.127
		500	0.0667	0.217
		725	0.0967	0.254
50	323.2	100	0.0133	0.021
		300	0.0400	0.096
		500	0.0667	0.159
		725	0.0967	0.222
65	338.2	100	0.0133	0.011
		300	0.0400	0.064
		500	0.0667	0.106
		725	0.0967	0.148

The compiler (HLC) added the Kelvin temperatures and the MPa pressures.

Auxiliary Information

Method/Apparatus/Procedure:
Static method. The apparatus is described in another paper.[1]

Source and Purity of Material:
(1) Fluoroethene. Source not given. Stated to be 99.9% pure.
(2) 2-(2-Furanyl)-1,3-dioxolane. Nothing specified.

Estimated Error:
Nothing specified.

Components:
(1) Fluoroethene or vinyl fluoride; C_2H_3F; [75-02-5]
(2) 1,1-Difluoroethane; $C_2H_4F_2$; [75-37-6]

Original Measurements:
Kh. U. Usamanov, T. S. Sirlibaev, A. A. Yul'chibaev, and E. F. Narkhodzhaev, Dep. Document **1975** VINITI 484-75.

Variables:
T/K = 283.2–313.2
p_1 /MPa = 0.203–1.520

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

The mole fraction solubility of fluoroethene in 1,1-difluoroethane at temperatures between 10 °C and 40 °C and pressures between 2.0 atm and 15.0 atm

Temperature		Pressure		Mol Fraction
(t/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	x_1
10	283.2	2.0	0.203	0.086
		5.0	0.507	0.242
		8.0	0.811	0.386
		10.0	1.013	0.493
		12.0	1.216	0.610
		15.0	1.520	0.741
20	293.2	2.0	0.203	0.048
		5.0	0.507	0.147
		8.0	0.811	0.292
		10.0	1.013	0.382
		12.0	1.216	0.462
		15.0	1.520	0.582
30	303.2	2.0	0.203	0.054
		5.0	0.507	0.131
		8.0	0.811	0.228
		10.0	1.013	0.310
		12.0	1.216	0.372
		15.0	1.520	0.463
40	313.2	2.0	0.203	0.047
		5.0	0.507	0.137
		8.0	0.811	0.213
		10.0	1.013	0.267
		12.0	1.216	0.318
		15.0	1.520	0.392

The compiler (HLC) added the Kelvin temperatures and the MPa pressures.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is described in another paper.[1]
The pressure has been identified above as the partial pressure of the fluoroethene, but it may be the total pressure.

Source and Purity of Material:
(1) Fluoroethene. Nothing specified.
(2) 1,1-Difluoroethane. Nothing specified.

Estimated Error:
Nothing specified.

References:
[1]E. R. Shenderei, Ya. D. Zel'venskii, and F. P. Ivanovskii, Khim. Prom. **No. 5**, 370 (1960).

Components:
(1) Fluoroethene or vinyl fluoride; C_2H_3F; [75-02-5]
(2) *N*-Methyl-2-pyrrolidinone; C_5H_9NO; [872-50-4]

Original Measurements:
Kh. U. Usamanov, T. S. Sirlibaev, A. A. Yulchibaev, and E. F. Narkhodzhaev, Dep. Document **1975** VINITI 484-75.

Variables:
T/K = 283.2–313.2
p_1 /MPa = 0.152–0.608

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

The mole fraction solubility of fluoroethene in *N*-methyl-2-pyrrolidinone at temperatures between 10 °C and 40 °C and pressures between 1.5 atm and 6.0 atm

Temperature		Pressure		Mol Fraction
(t/°C)	(T/K)	(p_1 /atm)	(p_1 /MPa)	x_1
10	283.2	1.5	0.152	0.250
		2.0	0.203	0.371
		2.5	0.253	0.528
		3.0	0.304	0.965
20	293.2	1.5	0.152	0.223
		2.0	0.203	0.256
		2.5	0.253	0.348
		3.0	0.304	0.352
		4.0	0.405	0.872
30	303.2	1.5	0.152	0.103
		2.0	0.203	0.161
		2.5	0.253	0.169
		3.0	0.304	0.280
		4.0	0.405	0.412
		5.0	0.507	0.590
40	313.2	1.5	0.152	0.074
		2.0	0.203	0.129
		2.5	0.253	0.147
		3.0	0.304	0.223
		4.0	0.405	0.319
		5.0	0.507	0.433
		6.0	0.608	0.542

The compiler (HLC) added the Kelvin temperatures and the MPa pressures.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is described in another paper.[1] The pressure has been identified above as the partial pressure of the fluoroethene, but it may be the total pressure.

Source and Purity of Material:
(1) Fluoroethene. Nothing specified.
(2) *N*-Methyl-2-pyrrolidinone. Nothing specified.

Estimated Error:
Nothing specified.

References:
[1]E. R. Shenderei, Ya. D. Zel'venskii, and F. P. Ivanovskii, Khim. Prom. **No. 5**, 370 (1960).

3.21. Hexafluoropropene

Components:
(1) Hexafluoropropene; C_3F_6; [116-15-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, and G. P. Kostyk, Dep. Document **1982**, VINITI 1733-82.

Variables:
T/K = 283.15–333.15
p_1 /MPa = 0.0400–0.1360

Prepared By:
Y. P. Yampol'skii and H. L. Clever

Experimental Values

Solubility of C_3F_6 in H_2O at temperatures between 283.15 K and 333.15 K and a partial pressure of 0.1013 MPa

Temperature (t/°C)	Temperature (T/K)	Mol Fraction $10^4 x_1$	Ostwald Coefficient (L/cm^3 cm^{-3})
10	283.15	0.351	0.0453
20	293.15	0.262	0.0349
30	303.15	0.194	0.0267
40	313.15	0.157	0.0222
50	323.15	0.127	0.0185
60	333.15	0.104	0.0155

The Kelvin temperatures and the Ostwald coefficients were added by the compiler (HLC). The authors report a heat of sorption of 4.53 kcal mol^{-1} (19.0 kJ mol^{-1}).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is described in the literature.[1]

Source and Purity of Material:
(1) Hexafluoropropene. Stated to be chromatographically pure.
(2) Water. Distilled.

Estimated Error:
Nothing specified.

References:
[1]G. E. Braude, I. L. Leites, and I. Z. Ddova, Khim. Prom. **No. 4**, 232 (1961).

Components:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene; C_3F_6; [116-15-4]
(2) N,N-Diethyl ethanesulfonamide; $C_6H_{15}NO_2S$; [33718-39-7]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, and F. B. Moin, Zh. Fiz. Khim. **52**(2), 495 (1978); Dep. Doc. VINITI No. 2464 (1977).

Variables:
T/K = 253.2–338.2
p_1 /MPa = 0.0133–0.0960

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Temperature (t/°C)	Temperature (T/K)	Pressure (p_1 /mmHg)	Pressure (p_1 /MPa)	Mol Fraction x_1
−20	253.2	100	0.0133	0.0085
		300	0.0400	0.0168
		500	0.0667	0.0346
		720	0.0960	0.0605
0	273.2	100	0.0133	0.0067
		300	0.0400	0.0120
		500	0.0667	0.0212
		720	0.0960	0.0390
20	293.2	100	0.0133	0.0050
		300	0.0400	0.0099
		500	0.0667	0.0162
		720	0.0960	0.0284
35	308.2	100	0.0133	0.0037
		300	0.0400	0.0086
		500	0.0667	0.0147
		720	0.0960	0.0252
50	323.2	100	0.0133	0.0024
		300	0.0400	0.0071
		500	0.0667	0.0130
		720	0.0960	0.0199
65	338.2	100	0.0133	0.0012
		300	0.0400	0.0057
		500	0.0667	0.0114
		720	0.0960	0.0170

Auxiliary Information

Method/Apparatus/Procedure:
Few details given.
The authors state that departures from Henry's law are probably due to weak donor-acceptor complexes.

Source and Purity of Material:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene.
(2) N,N-diethyl ethanesulfonamide.
Both components stated to be >98%.

Estimated Error:
Nothing specified.

Components:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene; C_3F_6 ; [116-15-4]
(2) *N*,*N*-Dimethyl ethanesulfonamide; $C_4H_{11}NO_2S$; [6338-68-7]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, and F. B. Moin, Zh. Fiz. Khim. **52**(2), 495 (1978); Dep. Doc. VINITI No. 2464 (1977).

Variables:
T/K = 293.2 – 338.2
p_1 /MPa = 0.0133 – 0.0960

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Solubility of 1,1,2,3,3,3-hexafluoro-1-propene in *N*,*N*-dimethyl ethanesulfonamide from 293.2 K to 338.2 K at partial pressures between 0.0133 MPa and 0.0960 MPa

Temperature		Pressure		Mole Fraction
(t/°C)	(T/K)	(p_1 /mmHg)	(p_1 /MPa)	x_1
20	293.2	100	0.0133	0.0049
		300	0.0400	0.0098
		500	0.0667	0.0147
		725	0.0967	0.0185
35	308.2	100	0.0133	0.0038
		300	0.0400	0.0086
		500	0.0667	0.0133
		725	0.0967	0.0170
50	323.2	100	0.0133	0.0028
		300	0.0400	0.0071
		500	0.0667	0.0119
		725	0.0967	0.0141
65	338.2	100	0.0133	0.0018
		300	0.0400	0.0062
		500	0.0667	0.0106
		725	0.0967	0.0141

Auxiliary Information

Method/Apparatus/Procedure:
Few details given.
The authors state that departures from Henry's law are probably due to weak donor-acceptor complexes.

Source and Purity of Material:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene.
(2) *N*,*N*-dimethyl ethanesulfonamide.
Both components stated to be >98%

Estimated Error:
Nothing specified.

Components:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene; C_3F_6 ; [116-15-4]
(2) Tetraethyl sulfamide; $C_8H_{20}N_2O_2S$; [2832-49-7]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, and F. B. Moin, Zh. Fiz. Khim. **52**(2), 495 (1978); Dep. Doc. VINITI No. 2464 (1977).

Variables:
T/K = 273.2 – 338.2
p_1 /MPa = 0.0133 – 0.0973

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Solubility of 1,1,2,3,3,3-hexafluoro-1-propene in tetraethyl sulfamide from 273.2 K to 338.2 K at partial pressures from 0.0133 MPa to 0.0973 MPa

Temperature		Pressure		Mole Fraction
(t/°C)	(T/K)	(p_1 /mmHg)	(p_1 /MPa)	x_1
0	273.2	100	0.0133	0.0121
		300	0.0400	0.0273
		500	0.0667	0.0388
		730	0.0967	0.0706
20	293.2	100	0.0133	0.0082
		300	0.0400	0.0222
		500	0.0667	0.0319
		730	0.0967	0.0456
35	308.2	100	0.0133	0.0063
		300	0.0400	0.0157
		500	0.0667	0.0234
		730	0.0967	0.0354
50	323.2	100	0.0133	0.0046
		300	0.0400	0.0131
		500	0.0667	0.0151
		730	0.0967	0.0210
65	338.2	100	0.0133	0.0030
		300	0.0400	0.0088
		500	0.0667	0.0131
		730	0.0967	0.0175

Auxiliary Information

Method/Apparatus/Procedure:
Few details given.
The authors state that departures from Henry's law are probably due to weak donor-acceptor complexes.

Source and Purity of Material:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene.
(2) Tetraethyl sulfamide.
Both components stated to be >98%.

Estimated Error:
Nothing specified.

Components:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene; C_3F_6; [116-15-4]
(2) *N*,*N*-Dimethyl methanesulfonamide; $C_5H_{13}NO_2S$; [2374-61-0]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, and F. B. Moin, Zh. Fiz. Khim. **52**(2), 495 (1978); Dep. Doc. VINITI No. 2464 (1977).

Variables:
T/K = 253.2–338.2
p_1 /MPa = 0.0133–0.0973

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Temperature (t/°C)	Temperature (T/K)	Pressure (p_1 /mmHg)	Pressure (p_1 /MPa)	Mole Fraction x_1
−20	253.2	100	0.0133	0.0079
		300	0.0400	0.0167
		500	0.0667	0.0346
		730	0.0973	0.0474
0	273.2	100	0.0133	0.0061
		300	0.0400	0.0118
		500	0.0667	0.0212
		730	0.0973	0.0249
20	293.2	100	0.0133	0.0046
		300	0.0400	0.0091
		500	0.0667	0.0162
		730	0.0973	0.0180
35	308.2	100	0.0133	0.0033
		300	0.0400	0.0086
		500	0.0667	0.0147
		730	0.0973	0.0140
50	323.2	100	0.0133	0.0021
		300	0.0400	0.0063
		500	0.0667	0.0130
		730	0.0973	0.0114
65	338.2	100	0.0133	0.0010
		300	0.0400	0.0050
		500	0.0667	0.0114
		730	0.0973	0.0100

Auxiliary Information

Method/Apparatus/Procedure:
Few details given.
The authors state that departures from Henry's law are probably due to weak donor-acceptor complexes.

Source and Purity of Material:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene.
(2) *N*,*N*-Dimethyl methanesulfonamide.
Both components stated to be >98%.

Estimated Error:
Nothing specified.

Components:
(1) 1,1,2,3,3,3-Hexafluoro-1-propene; C_3F_6; [116-15-4] (2) 2-Methylpyrrolidone; C_5H_9NO; [872-50-4]

Original Measurements:
V. M. Yakovlev, I. D. Kushina, A. M. Koval'skaya, and T. I. Politanskaya, Zh. Prikl. Khim. **55**, 1325–1330 (1982); Russ. J. Appl. Chem. (Eng. Transl.) **55**, 1216–1220 (1982).

Variables:
T/K = 273.15–393.15
p_1 /MPa = 0.0966

Prepared By:
H. L. Clever

Experimental Values

Absorption coefficient of 1,1,2,3,3,3-hexafluoro-1-propene in 2-methylpyrrolidone from 273.15 K to 393.15 K at a partial pressure of 0.0966 MPa

Temperature (t/°C)	Temperature (T/K)	Absorption Coefficient (β/mL mL^{-1})
0	273.15	2.26
20	293.15	1.36
40	313.15	0.9
70	343.15	0.63
120	393.15	0.46

The compiler added the Kelvin temperatures.
The authors used three data points to determine the coefficients of an Antoine type equation.

$$\ln \beta = -1.6894 + [172.3874/(68.82 + t/°C)]$$

Henry's constant, $K_H = f_1 / x_1$, and the enthalpy of solution are shown in figures as functions of temperature. The enthalpy of solution is about 14 kcal mol^{-1} (59 kJ mol^{-1} at 293 K).

Auxiliary Information

Method/Apparatus/Procedure:
The solubility coefficients were determined in an apparatus for static[1] and for dynamic[2] absorption in vessels of small volume. Rapid establishment of equilibrium was achieved by mechanical stirring or by bubbling. The experiments were conducted at a pressure of 966 hPa (0.0966 MPa) over the 0–120 °C temperature interval. A vapor pressure equation for 2-methylpyrrolidone is given.

Source and Purity of Material:
(1) 1,1,2,3,3,3-Hexafluoropropene. Nothing specified.
(2) 2-Methylpyrrolidone. Source not given. Vacuum distilled, water content <0.2 mass %.

Estimated Error:
δT/K = 0.5
$\delta\beta/\beta$ = 0.05 (compiler).

References:
[1]R. G. Makitra, G. I. Politanskaya, and F. B. Moin, Zh. Prikl. Khim. **52**, 2623 (1979).
[2]I. R. Krichevskii and M. V. Koroleva, Zh. Fiz. Khim. **15**, 327 (1941).

3.22. Oxy*bis*(trifluoromethane)

Components:
(1) Oxy*bis*(trifluoromethane); C_3F_6O; [1479-49-8]
(2) Tetraethyl sulfamide; $C_8H_{20}N_2O_2S$; [2832-49-7]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, and F. B. Moin, Zh. Fiz. Khim. **52**(2), 495 (1978); Dep. Doc. VINITI No. 2464 (1977).

Variables:
T/K = 273.2–338.2
p_1 /MPa = 0.0133–0.0973

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Solubility of oxy*bis*(trifluoromethane) in tetraethyl sulfamide from 273.2 K to 338.2 K at partial pressures from 0.0133 MPa to 0.0973 MPa

Temperature		Pressure		Mole Fraction
(t/°C)	(T/K)	(p_1 /mmHg)	(p_1 /MPa)	x_1
0	273.2	100	0.0133	0.0105
		300	0.0400	0.0206
		500	0.0667	0.0355
		730	0.0973	0.0532
20	293.2	100	0.0133	0.0066
		300	0.0400	0.0146
		500	0.0667	0.0273
		730	0.0973	0.0411
30	308.2	100	0.0133	0.0048
		300	0.0400	0.0111
		500	0.0667	0.0218
		730	0.0973	0.0354
50	323.2	100	0.0133	0.0031
		300	0.0400	0.0092
		500	0.0667	0.0195
		730	0.0973	0.0313
65	338.2	100	0.0133	0.0015
		300	0.0400	0.0073
		500	0.0667	0.0175
		730	0.0973	0.0272

Auxiliary Information

Method/Apparatus/Procedure:
Few details given.
The authors state that departures from Henry's law are probably due to weak donor-acceptor complexes.

Source and Purity of Material:
(1) Oxy*bis*(trifluoromethane) or hexafluoro dimethyl ether.
(2) Tetraethyl sulfamide.
Both components stated to be >98%.

Estimated Error:
Nothing specified.

Components:
(1) Oxy*bis*(trifluoromethane); C_3F_6O; [1479-49-8]
(2) *N*,*N*-Dimethyl ethanesulfonamide; $C_4H_{11}NO_2S$; [6338-68-7]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, and F. B. Moin, Zh. Fiz. Khim. **52**(2), 495 (1978); Dep. Doc. VINITI No. 2464 (1977).

Variables:
T/K = 293.2–338.2
p_1/MPa = 0.0133–0.0960

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Solubility of oxy*bis*(trifluoromethane) in *N*,*N*-dimethyl ethane-sulfonamide from 293.2 K to 338.2 K at partial pressure from 0.0133 MPa to 0.0960 MPa

Temperature		Pressure		Mole Fraction
(t/°C)	(T/K)	(p_1 /mmHg)	(p_1 /MPa)	x_1
20	293.2	100	0.0133	0.0039
		300	0.0400	0.0089
		500	0.0667	0.0127
		740	0.0987	0.0176
35	308.2	100	0.0133	0.0029
		300	0.0400	0.0065
		500	0.0667	0.0114
		740	0.0987	0.0152
50	323.2	100	0.0133	0.0018
		300	0.0400	0.0053
		500	0.0667	0.0119
		740	0.0987	0.0137
65	338.2	100	0.0133	0.0009
		300	0.0400	0.0036
		500	0.0667	0.0080
		740	0.0987	0.0115

Auxiliary Information

Method/Apparatus/Procedure:
Few details given.
The authors state that departures from Henry's law are probably due to weak donor-acceptor complexes.

Source and Purity of Material:
(1) Oxy*bis*(trifluoromethane).
(2) *N*,*N*-dimethyl ethanesulfonamide.
Both components stated to be >98%.

Estimated Error:
Nothing specified.

Components:
(1) Oxy*bis*(trifluoromethane); C_3F_6O; [1479-49-8]
(2) *N*,*N*-Diethyl ethanesulfonamide; $C_6H_{15}NO_2S$; [33718-39-7]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, and F. B. Moin, Zh. Fiz. Khim. **52**(2), 495 (1978); Dep. Doc. VINITI No. 2464 (1977).

Variables:
T/K = 253.2–338.2
p_1 /MPa = 0.0133–0.0987

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Temperature		Pressure		Mole Fraction
(t/°C)	(T/K)	(p_1 /mmHg)	(p_1 /MPa)	x_1
−20	253.2	100	0.0133	0.0141
		300	0.0400	0.0210
		500	0.0667	0.0306
		740	0.0987	0.0566
0	273.2	100	0.0133	0.0107
		300	0.0400	0.0172
		500	0.0667	0.0238
		740	0.0987	0.0489
20	293.2	100	0.0133	0.0063
		300	0.0400	0.0138
		500	0.0667	0.0184
		740	0.0987	0.0424
35	308.2	100	0.0133	0.0049
		300	0.0400	0.0123
		500	0.0667	0.0171
		740	0.0987	0.0289
50	323.2	100	0.0133	0.0036
		300	0.0400	0.0106
		500	0.0667	0.0153
		740	0.0987	0.0233
65	338.2	100	0.0133	0.0023
		300	0.0400	0.0091
		500	0.0667	0.0136
		740	0.0987	0.0181

Auxiliary Information

Method/Apparatus/Procedure:
Few details given.
The authors state that departures from Henry's law are probably due to weak donor-acceptor complexes.

Source and Purity of Material:
(1) Oxy*bis*(trifluoromethane).
(2) *N*,*N*-Diethyl ethanesulfonamide.
Both components stated to be >98%.

Estimated Error:
Nothing specified.

Components:
(1) Oxy*bis*(trifluoromethane); C_3F_6O; [1479-49-8]
(2) *N*,*N*-Diethyl methanesulfonamide; $C_5H_{13}NO_2S$; [2374-61-0]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, and F. B. Moin, Zh. Fiz. Khim. **52**(2), 495 (1978).
Dep. Doc. VINITI No. 2464 (1977).

Variables:
T/K = 253.2–338.2
p_1 /MPa = 0.0133–0.0987

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Temperature		Pressure		Mole Fraction
t/°C	T/K	(p_1 /mmHg)	(p_1 /MPa)	x_1
−20	253.2	100	0.0133	0.0079
		300	0.0400	0.0116
		500	0.0667	0.0167
		730	0.0973	0.0329
0	273.2	100	0.0133	0.0061
		300	0.0400	0.0096
		500	0.0667	0.0129
		730	0.0973	0.0249
20	293.2	100	0.0133	0.0046
		300	0.0400	0.0068
		500	0.0667	0.0091
		730	0.0973	0.0201
35	308.2	100	0.0133	0.0033
		300	0.0400	0.0055
		500	0.0667	0.0086
		730	0.0973	0.0151
50	323.2	100	0.0133	0.0021
		300	0.0400	0.0042
		500	0.0667	0.0063
		730	0.0973	0.0125
65	338.2	100	0.0133	0.0010
		300	0.0400	0.0030
		500	0.0667	0.0050
		730	0.0973	0.0100

Auxiliary Information

Method/Apparatus/Procedure:
Few details given.
The authors state that departures from Henry's law are probably due to weak donor-acceptor complexes.

Source and Purity of Materials:
(1) Oxy*bis*(trifluoromethane).
(2) *N*,*N*-Diethyl methanesulfonamide.
Both components stated to be >98%.

Estimated Error:
Nothing specified.

3.23. Trifluoro(trifluoromethyl)oxirane

Components:
(1) Trifluoro(trifluoromethyl)oxirane; C_3F_6O; [428-59-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. G. Makitra, T. I. Politanskaya, F. B. Moin, and G. P. Kostyk, Dep. Doc. VINITI No. 1733–82 (1982).

Variables:
T/K = 283.2–333.2
p_1 /MPa = 0.1013

Prepared By:
Y. P. Yampolskii and H. L. Clever

Experimental Values

Solubility of trifluoro(trifluoromethyl)oxirane in water from 283.2 K to 333.2 K at a partial pressure of 0.1013 MPa

Temperature		Mole Fraction	Ostwald Coefficient
(t/°C)	(T/K)	$10^4 x_1$	(L/cm^3 cm^{-3})
10	283.2	0.246	0.0317
20	293.2	0.194	0.0259
30	303.2	0.142	0.0195
40	313.2	0.112	0.0131
50	323.2	0.090	0.0131
60	333.2	0.045	0.0067

The Kelvin temperatures and the kPa pressure values were added by the compiler (HLC). The authors conclude Henry's law is obeyed. The compiler (HLC) added the Kelvin temperatures and the Ostwald coefficients. The authors report a heat of absorption of 6.34 kcal mol^{-1} (26.5 kJ mol^{-1}).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is described in the Ref. 1

Source and Purity of Material:
(1) Trifluoro(trifluoromethyl)oxirane or hexafluoropropene oxide. Stated to be chromatographically pure.
(2) Water. Distilled.

Estimated Error:
Nothing specified.

References:
[1]G. E. Braude, I. L. Leites, and I. Z. Dedova, Khim. Prom. (No. 4), 232 (1961).

3.24. Tetrafluorosilane

Components:
(1) Tetrafluorosilane; SiF_4; [7783-01-1]
(2) Hydrogen fluoride; HF; [7664-39-3]

Original Measurements:
N. S. Nikolaev, Izv. Sektora Fiz.-Khim., Anal., Inst. Obshchei Neorg. Khim., Akad. Nauk SSSR **25**, 375–380 (1954); Chem. Abstr. **49**, 14436i (1955).

Variables:
T/K = 253–256

Prepared By:

Experimental Values

The solubility of SiF_4 in concentrated HF was studied. Only the abstract was available to the compiler. It states that at HF concentrations >96 wt % the SiF_4 solubility is >0.05 wt %. There is no mention of temperature or pressure in the abstract. Other information was taken from the compilation of Yu. P. Yampol'skii.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium was established in a thermostated silver vessel. Water solutions of HF were saturated with SiF_4. Liquid samples of the saturated solutions were withdrawn from the vessel and titrated with standard alkali with added KCl by the method described by Tananaev and Savchenko.[1]

Source and Purity of Material:
(1) Nothing specified for either component.
(2)

Estimated Error:
Nothing specified.

References:
[1]I. V. Tananaev and G. S. Savchenko, Zh. Prikl. Khim. **7**, 1071 (1934).

Components:
(1) Tetrafluorosilane; SiF_4; [7783-01-1]
(2) Hydrogen fluoride; HF; [7664-39-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
N. S. Nikolaev, Izv. Sektora Fiz.-Khim., Anal., Inst. Obshchei Neorg. Khim., Akad. Nauk SSSR **25**, 375–380 (1954).

Variables:
T/K = 253–256
$10^2 w_2$ /HF = 71.95–96.00

Prepared By:
Yu. P. Yampol'skii

Experimental Values

The $SiF_4 + HF + H_2O$ System at −20 °C to −17 °C. Composition by weight percent

HF $10^2 w_2$	H_2O $10^2 w_3$	SiF_4 $10^2 w_1$
71.95	20.00	7.95
73.18	19.30	7.52
73.25	19.60	7.10
78.15	17.30	4.55
80.00	16.65	3.35
84.50	13.75	1.75
88.05	10.85	1.09
91.30	8.30	0.42
92.05	7.25	0.68
93.40	6.35	0.28
95.50	4.35	0.15
96.00	4.00	0.05

The results indicate the existence of the equilibrium: $SiF_4(aq) + 2HF(aq) = H_2SiF_6(aq)$

See previous data sheet.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibrium was established in a thermostated silver vessel. Water solutions of HF were saturated with SiF_4. Liquid samples of the saturated solutions were withdrawn from the vessel and titrated with standard alkali with added KCl by the method described by Tananaev and Savchenko.[1]

Source and Purity of Material:
(1) Nothing specified for either component.
(2)

Estimated Error:
Nothing specified.

References:
[1] I. V. Tananaev and G. S. Savchenko, Zh. Prikl. Khim. **7**, 1071 (1934).

Components:
(1) Tetrafluorosilane; SiF_4; [7783-01-1]
(2) Alcohols, ketones, acids, etc. (See table below).
(3) Water; H_2O; [7732-18-5]

Original Measurements:
G. Tarbutton, E. P. Egan, Jr., and S. G. Frary, J. Am. Chem. Soc. **61**, 2555–2556 (1939).

Variables:
T/K = 300–306
p_1 /kPa = 99.99–101.325

Prepared By:
H. L. Clever

Experimental Values

Solubility of silicon tetrafluoride at room temperature (27 °C–33 °C) and a total pressure of 750–760 mmHg (0.100–0.1013) MPa

Solvent	g SiF_4 per 100 cm^3 Solvent	SiF_4 $10^2 w_1$
Methanol; CH_3OH; [67-56-1], absolute	–	32.8
Methanol + Water; 94 wt% CH_3OH	–	39.0
Ethanol; C_2H_5OH; [64-17-5], absolute	57.2	36.4
Ethanol + Water, 96.1 wt % C_2H_5OH	60.8	37.8
Ethanol + Water, 95 wt % C_2H_5OH	61.4	38.1
Ethanol + Water, 94.3 wt % C_2H_5OH	61.5	38.1
Ethanol + Water, 92.6 wt% C_2H_5OH	63.4	38.8
Ethanol + Water, 91.0 wt% C_2H_5OH	63.9	39.0
2-Propanol; C_3H_7OH; [67-63-0], 98 wt %	39.4	28.2
1-Butanol; C_4H_9OH; [71-36-3], 98 wt % (USP)	30.4	23.4
Amyl alcohols (fusel oil)[a]	20.9	17.3
1,2-Ethanediol (glycol); CH_2OHCH_2OH; [107-21-11]	–	26.2
2,2′-Oxybis-ethanol (diethylene glycol); $C_4H_{10}O_3$; [111-46-6]	–	17.6
1,2,3-Propanetriol (glycerol); $C_3H_5(OH)_3$; [56-81-5]	–	5.7
2-Propanone (acetone); CH_3COOH_3; [67-64-1]	3.2	3.1
Acetic acid, glacial; CH_3COOH; [64-19-7]	1.1	1.1
2-Oxo-propanoic acid (pyruvic acid); $C_3H_4O_3$; [127-17-5]	–	4.4
Benzene; C_6H_6; [71-43-2]	b	b
1,1,2-Trichloroethene; C_2HCl_3; [79-01-1]	b	b
Tetrachloromethane; CCl_4; [56-23-5]	c	c

[a] A purified fusel oil that is about 85 wt % 3-methyl-1-butanol; $C_3H_{11}OH$; [123-51-3] and 15 wt % 2-methyl-1-butanol; $C_5H_{11}OH$; [137-32-6].
[b] Sparingly soluble.
[c] Insoluble.

The authors state the saturated solutions remain clear, showing no precipitation of silica, when allowed to stand overnight out of direct contact with air.

Compiler's Note: Tetrafluorosilane dissolves in and reacts with water. The products of the reaction vary with the SiF_4 concentration in water and temperature. Products include H_2SiF_6, HSi_2O_2F, HF, and others. Some of the solvents in this study contained a known amount of water, other solvents may have had trace amounts of water present and these reactions may be occurring in these systems.

In addition to the solubility values the authors describe other qualitative experiments on several of these solutions. See the original paper for details.

Auxiliary Information

Method/Apparatus/Procedure:

The saturated solutions were prepared by circulating the purified SiF_4 gas through the various solvents, contained in an absorption tower or an Orsat pipet, in a closed system at atmospheric pressure until saturation appeared to be attained. The concentration of SiF_4 in the saturated solution was calculated from the fluorine content of weighed samples determined by an analytical method. No details of the method were given.

Source and Purity of Material:

(1) Tetrafluorosilane. No information other than to state it was a purified gas.
(2) Solvents were used as purchased except the absolute ethanol, which was purified. Solvents specified to be chemical pure (c. p.) were the glycol, diethylene glycol, glycerol, and acetone. Specified as USP quality were the 95% ethanol and the 1-butanol.

Estimated Error:

Neither temperature nor pressure were well controlled. The solubility values may be useful, but they are of marginal quality.

4. System Index

Pages preceded by E refer to evaluation texts, whereas those not preceded by E refer to compilation tables.

Editor-in-Chief's note: Periodically, the reader will note the entry (0C-6-11) for sulfur hexafluoride; SF_6; along with the CAS Registry number [2551-62-4]. The (OC-6-11)-sulfur fluoride, SF_6, designation is the Chemical Abstracts Service Index name given in the CA Registry Index. It also used with XeF_6; (OC-6-11)-xenon fluoride.

4.1. Solute Index

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Benzene, 1,3-dimethyl-	+ borane, trifluoro-(mixed solvent with HF)	E214, 221
	+ methane, tetrafluoro-	312
	+ sulfur fluoride, (OC-6-11)-	259
Benzene, 1,4-dimethyl-	+ borane, trifluoro-(mixed solvent with HF)	E214, 221
	+ ethane, fluoro-	386
	+ methane, tetrafluoro-	312
	+ sulfur fluoride, (OC-6-11)-	260
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Benzene, nitro-	+ borane, trifluoro-	223
	+ sulfur fluoride, (OC-6-11)-	282
Benzene, pentamethyl-	+ borane, trifluoro- (mixed solven with HF)	E214
Benzene, 1,2,3,4-tetramethyl-	+ borane, trifluoro- (mixed solvent with HF)	E214
Benzene, 1,2,3,5-tetramethyl-	+ borane, trifluoro- (mixed solvent with HF)	E214
Benzene, 1,3,4,5-tetramethyl-	+ borane, trifluoro- (mixed solvent with HF)	E214
Benzene, 1,2,3-tirmethyl-	+ borane, trifluoro- (mixed solvent with HF)	E214
Benzene, 1,2,4-tetramethyl-	+ borane, trifluoro- (mixed solvent with HF)	E214
Benzene, 1,3,5-tetramethyl-	+ borane, trifluoro- (mixed solvent with HF)	E214
Benzonitrile	+ sulfur fluoride, (OC-6-11)-	282
1,1′-Bicyclohexyl	+ sulfur fluoride, (OC-6-11)-	257
Biolayers, lipid	+ ethane, hexafluoro-	345
	+ methane, tetrafluoro-	301
	+ sulfur fluoride, (OC-6-11)-	235
Blood, dog, components, and tissues	+ sulfur fluoride, (OC-6-11)-	234, 287
Blood, human, components, and tissues	+ sulfur fluoride, (OC-6-11)-	245, 288, 289
Blood, rabbit, components, and tissues	+ sulfur fluoride, (OC-6-11)-	287
Blood, rat, components, and tissues	+ ethane, 1,1-difluoro-	408
	+ methane, difluoro-	332

	+ sulfur fluoride, (OC-6-11)-	289
Bone (semi-wet)	+ methane, fluoro-	341
Bromine trifluoride	+ xenon fluoride, XeF_2 (qualitative observation)	E205–206
	+ xenon fluoride, XeF_4 (qualitative observation)	E205–206
Buffer, phosphate	+ sulfur fluoride, (OC-6-11)-	286
Buffer, tris HCl	+ ethane, hexafluoro-	345
	+ methane, tetrafluoro-	301
	+ sulfur fluoride, (OC-6-11)-	235
Butanamine, 1,1,2,2,3,3,4,4,4-nonafluoro-*N*, *N*-*bis*(nonafluorobutyl)-1-	+ cyclobutane, octafluoro-	399
	+ ethane, hexafluoro-	348
	+ methane, tetrafluoro-	325
	+ sulfur fluoride, (OC-6-11)-	283
1-Butanol	+ ethane, fluoro-	387
	+ methane, fluoro-	343
	+ methane, tetrafluoro-	313–314
	+ silane, tetrafluoro-	419–420
	+ sulfur fluoride, (OC-6-11)-	233, 260–261
1-Butanol, 2-methyl-(amyl alcohol component, 15%)	+ silane, tetrafluoro-	419–420
1-Butanol, 3-methyl-(amyl alcohol component, 85%)	+ silane, tetrafluoro-	419–420
2-Butanol	+ methane, tetrafluoro-	315
	+ sulfur fluoride, (OC-6-11)-	262
Carbon disulfide	+ cyclobutane, octafluoro-	399
	+ methane, tetrafluoro-	291, 328
	+ sulfur fluoride, (OC-6-11)-	278–279
Chlorex, see ethane, 1,1′-oxy(*bis*), 2-chloro-		
CTAB, see hexadecanaminium, *N*,*N*,*N*-trimethyl-, bromide (aqueous)		
Cyclobutane, octafluoro-	+ ethane, tetrafluoro-	405
Cycloheptanone	+ methane, tetrafluoro-	319
	+ sulfur fluoride, (OC-6-11)-	268
Cyclohexane	+ cyclobutane, octafluoro-	397
	+ ethane, hexafluoro-	345
	+ methane, tetrafluoro-	306
	+ propane, octafluoro-	392
	+ sulfur fluoride, (OC-6-11)-	252–253
Cyclohexane, bromo-	+ methane, tetrafluoro-	325
	+ sulfur fluoride, (OC-6-11)-	278
Cyclohexane, chloro-	+ methane, tetrafluoro-	326
	+ sulfur fluoride, (OC-6-11)-	273
Cyclohexane, decafluoro*bis*(trifluoromethyl)-	+ sulfur fluoride, (OC-6-11)-	276
Cyclohexane, 1,2-dimethyl-, *cis*-	+ methane, tetrafluoro-	307
	+ sulfur fluoride, (OC-6-11)-	254
Cyclohexane, 1,2-dimethyl-, *trans*-	+ methane, tetrafluoro-	308
	+ sulfur fluoride, (OC-6-11)-	254
Cyclohexane, 1,3-dimethyl-, *cis*- and *trans*-mixture	+ methane, tetrafluoro-	308
	+ sulfur fluoride, (OC-6-11)-	255
Cyclohexane, 1,4-dimethyl-, *cis*- and *trans*-mixture	+ methane, tetrafluoro-	309
	+ sulfur fluoride, (OC-6-11)-	255
Cyclohexane, methyl-	+ methane, tetrafluoro-	307
	+ sulfur fluoride, (OC-6-11)-	253
Cyclohexanone	+ ethane, fluoro-	388
	+ methane, tetrafluoro-	318
	+ sulfur fluoride, (OC-6-11)-	267
Cyclohexanone, 2,6-dimethyl-	+ methane, tetrafluoro-	320
	+ sulfur fluoride, (OC-6-11)-	268
Cyclohexanone, 2-methyl-	+ methane, tetrafluoro-	319
	+ sulfur fluoride, (OC-6-11)-	267
Cyclooctane	+ methane, tetrafluoro-	309
	+ sulfur fluoride, (OC-6-11)-	252, 256
Cyclopentane	+ sulfur fluoride, (OC-6-11)-	252
Cyclopentanone	+ methane, tetrafluoro-	318
	+ sulfur fluoride, (OC-6-11)-	266
Cyclotetrasiloxane, octamethyl-	+ sulfur fluoride, (OC-6-11)-	285

Decanaminium, *N*,*N*,*N*-trimethyl-, bromide (aqueous)	+ methane, tetrafluoro-	E298, 299
Decane	+ methane, tetrafluoro-	302–303, 305
	+ sulfur fluoride, (OC-6-11)-	247–248, 251
1-Decanol	+ methane, tetrafluoro-	313, 316
	+ sulfur fluoride, (OC-6-11)-	260–261, 264
Diethyl carbonate	+ methane, tetrafluoro-	323
Diethylene glycol, see ethanol, 2,2-oxy*bis*-		
Dimethyl carbonate	+ methane, tetrafluoro-	323
Dimethylsulfoxide, see methane,1,1-sulfinyl*bis*-		
1,4-Dioxane	+ cyclobutane, octafluoro-	398
	+ ethane, fluoro-	383
	+ ethane, fluoro-	388
	+ ethene, fluoro-	411
	+ methane, tetrafluoro-	317
	+ sulfur fluoride, (OC-6-11)-	269, 282
	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
1,3-Dioxan	+ xenon fluoride, XeF_2 (Qualitative observation)	E205-E206
1,3-Dioxolane-2-one, 4-methyl-	+ sulfur fluoride, (OC-6-11)-	266
1,3-Dioxolane, 2-(2-furanyl)-	+ ethane, fluoro-	411
Dodecane	+ methane, tetrafluoro-	302–303
	+ sulfur fluoride, (OC-6-11)-	247–248
DTAB, see decanaminium, *N*,*N*,*N*-trimethyl-, bromide		
Eicosane	+ ethane, 1,1-difluoro-	379
	+ ethane, pentafluoro-	350
	+ 1,1,1,2-tetrafluoro-	358
	+ 1,1,1-trifluoro-	373
Electrolytes (aqueous)	+ methane tetrafluoro-	E298
	+ sulfur fuoride, (OC-6-11)-	E240–E241
Ethanaminium, *N*,*N*,*N*-triethyl-, bromide (aqueous)	+ sulfur fluoride, (OC-6-11)-	E240–E241, 244
Ethane, 1,2-dibromo-1,1,2,2-tetrachloro-	+ ethene, tetrafluoro-	404
Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-	+ sulfur fluoride, (OC-6-11)-	275
Ethane, 1,1-difluoro-	+ ethene, fluoro-	412
	+ methane, trifluoro-	330
Ethane, 1,1′-[methylene*bis*(oxy)]*bis*-	+ methane, tetrafluoro-	320
	+ sulfur fluoride, (OC-6-11)-	271
Ethane, 1,1′oxy(*bis*)-, 2-chloro-	+ borane, trifluoro-	223
Ethane, 1,1′oxy(*bis*)(2-methoxy)-	+ ethane, fluoro-	388
Ethane, 1,1′-oxy*bis*-	+ xenon fluoride, XeF_4 (qualitative observation)	E205–E206
Ethane, pentafluoro-	+ methane, difluoro-	337
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-	+ ethane, hexafluoro-	346-347
	+ ethene, tetrafluoro-	403
	+ sulfur fluoride, (OC-6-11)-	274–275
Ethane, 1,1,1-trifluoro-	+ methane, tetrafluoro-	331
1,2-Ethanediol	+ ethane, fluoro-	387
	+ silane, tetrafluoro-	419–420
Ethanol	+ ethane, 1,1-difluoro-	381
	+ ethane, fluoro-	387
	+ ethane, pentafluoro-	351–352
	+ ethane, 1,1,1,2-tetrafluoro-	359–360
	+ ethene, difluoro-	408
	+ ethene, fluoro-	409
	+ methane, difluoro-	334
	+ methane, fluoro-	342
	+ methae, tetrafluoro-	291, 313
	+ silane, tetrafluoro-	419–420
	+ sulfur fluoride, (OC-6-11)-	233, 260–261, 263, 293
Ethanol (aqueous)	+ silane, tetrafluoro-	419–420
Ethanol, 2,2-oxy*bis*-	+ silane, tetrafluoro-	419–420
Ethanol, ,2,2′-[oxy*bis*(2,1-ethanediyloxy)]*bis*-	+ ethane, 1,1,1,2-terafluoro-	366
Ethanol, 2,2,2-triflroro-	+ methane, tetrafluoro-	323
	+ sulfur fluoride, (OC-6-11)-	246, 265
Ethanol, 2,2,2-trifluoro-(aqueous)	+ methane, tetrafluoro-	301
Ethene, 1,1,2-trichloro-	+ silane, tetrafluoro-(qualitative observation)	419–420
Fluorocarbon, commercial product FC-75, 3M Co.	+ sulfur fluoride, (OC-6-11)-	277

Fluorocarbon, commercial product FC-88, 3M Co.	+ sulfur fluoride, (OC-6-11)-	277
Formaldehyde diethyl acetal, see ethane, 1,1′-[methylene-*bis*(oxy)]*bis*-		
Formamide, *N*-methyl-	+ sulfur fluoride, (OC-6-11)-	282
Formamide, *N*,*N*-dimethyl-	+ ethane, fluoro-	389
	+ sulfur fluoride, (OC-6-11)-	282
	+ xenon fluoride, XeF_2 (qualitative obsevation)	E205–E206
	+ xenon fluoride, XeF_4 (qualitative observation)	E205–E206
Furan, tetrahydro-	+ ethane, fluoro-	387
	+ methane, tetrafluoro-	321
	+ sulfur fluoride, (OC-6-11)-	270
	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
Furan, tetrahydro-2-methyl-	+ methane, tetrafluoro-	321
	+ sulfur fluoride, (OC-6-11)-	271
D-Glucose (aqueous)	+ sulfur fluoride, (OC-6-11)-	236
Glycerol, see 1,2,3-propanetriol		
Heptane	+ ethane, fluoro-	385
	+ methane, tetrafluoro-	302–303
	+ sulfur fluoride, (OC-6-11)-	247–248
1-Heptanol	+ methane, tetrafluoro-	313
	+ sulfur fluoride, (OC-6-11)-	233, 260–261
Hexadecanaminium, *N*,*N*,*N*-trimethyl-, bromide (aqueous)	+ methane, tetrafluoro-	E298, 299
Hexadecane	+ ethane, 1,1-difluoro-	378
	+ ethane, pentafluoro-	349
	+ ethane, 1,1,1,2-tetrafluoro-	357
	+ ethane, 1,1,1-trifluoro-	372
	+ methane, tetrafluoro-	302–303
	+ sulfur fluoride, (OC-6-11)-	247–248
Hexamethylene oxide, see oxepane		
Hexamethylphosphoric triamide	+ sulfur fluoride, (OC-6-11)-	281
Hexane	+ methane, tetrafluoro-	302–303
	+ sulfur fluoride, (OC-6-11)-	247–248, 250
1-Hexanol	+ methane, tetrafluoro-	313
	+ sulfur fluoride, (OC-6-11)-	233, 260–261
Hexene, dodecafluoro-(isomer mixture)	+ ethene, tetrafluoro-	405
	+ sulfur fluoride, (OC-6-11)-	276
Hexene, 1,1,2,2,3,3,4,4,5,5,6,6-dodecafluoro-1, 6-*bis*(tri-fluoromethoxy)-	+ ethene, tetrafluoro-	407
Hydrazine, methyl-	+ sulfur fluoride, (OC-6-11)-	281
Hydrogen chloride (aqueous)	+ ethene, tetrafluoro-	401
	+ sulfur fluoride, (OC-6-11)-	E240–E241, 242
Hydrogen fluoride	+ borane, trifluoro-	E214 215–217, 221
	+ nitrogen fluoride, NF_3	227
	+ silane, tetrafluoro-(aqueous)	418–419
	+ xenon fluoride, XeF_2	E205–E206, 209–210
	+ xenon fluoride, XeF_4	E205–E206, 211
	+ xenon fluoride, (OC-6-11)-, XeF_6	E205–E206, 210
Hydrogen fluoride + Nitrosyl fluoride (3:1 mixture)	+ xenon fluoride, XeF_2	E205–E206, 211
	+ xenon fluoride, XeF_4	E205–E206, 211
Iodine pentafluoride	+ xenon fluoride, XeF_4	E205–E206, 212
	+ xenon fluoride, XeF_4	E205–E206, 212
IPH (perfluorohexene isomer mixture), see hexane, Dodecafluoro-, (isomer mixture)		
Isooctane, see pentane, 2,2,4-trimethyl-		
Lithium chloride (aqueous)	+ sulfur fluoride, (OC-6-11)-	E240–E241, 243
Lithium salt of nonadecafluorodecanoic acid (aqueous)	+ methane, tetrafluoro-	E298, 300
Lubricating oils (commercial)	+ ethane, 1,1,1,2-tetrafluoro-	371
Lung, human, homogenate	+ sulfur fluoride, (OC-6-11)-	285
Methanaminium, *N*,*N*,*N*-trimethyl-, iodide (aqueous)	+ sulfur fluoride, (OC-6-11)-	E240–E241, 244
Methane, chlorotrifluoro-	+ methane, tetrafluoro-	326
	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
Methane, dichlorodifluoro-	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
	+ xenon fluoride, XeF_4 (qualitative observation)	E205–E206

Methane, fluorotrichloro-	+ xenon fluoride, XeF_2 (qualitative observation)	Not listed
	+ xenon fluoride, XeF_4 (qualitative observation)	E205–E206
Methane, nitro-	+ sulfur fluoride, (OC-6-11)-	230, 280
	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
Methane, 1,1-sulfinyl*bis*-	+ ethane, fluoro-	389
	+ sulfur fluoride, (OX-6-11)-	279
	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
	+ xenon fluoride, XeF_4 (qualitative observation)	E205–E206
Methane, tetrachloro-	+ ethane, fluoro-	389
	+ methane, tetrafluoro-	90, 324, 327, 391
	+ silane, tetrafluoro-(qualitative observation)	419–420
	+ sulfur fluoride, (OC-6-11)-	272–273
	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
	+ xenon fluoride, XeF_4 (qualitative observation)	E205–E206
Methane, trichloro-	+ ethane, fluoro-	388
	+ ethane, 1,1-difluoro-	408
Methanol	+ ethane, 1,1-difluoro-	380
	+ ethane, pentafluoro-	350–351
	+ ethane, 1,1,1,2-tetrafluoro-	358–359
	+ methane, difluoro-	333
	+ methane, fluoro-	341
	+ methane, tetrafluoro-	313
	+ silane, tetrafluoro-	419–420
	+ sulfur fluoride, (OC-6-11)-	233, 260–261, 263
Methanol (aqueous)	+ silane, tetrafluoro-	419–420
Miscellaneous solvents	+ methane, tetrafluoro-(qualitative observations)	301
Naphthalene, decahydro-, *cis*-	+ sulfur fluoride, (OC-6-11)-	256
Naphthalene, decahydro-, *trans*-	+ sulfur fluoride, (OC-6-11)-	256
Nitric acid, potassium salt (aqueous)	+ sulfur fluoride, (OC-6-11)-	E240–E241, 244
Nitrogen oxide, NO	+ Borane, trifluoro-	218
	+ sulfur fluoride, (OC-6-11)-	218
Nitrogen oxide, N_2O_4	+ sulfur fluoride, (OC-6-11)-	280
Nitrous acid, sodium salt (aqueous)	+ sulfur fluoride, (OC-6-11)-	E240–E241, 245
Nonane	+ methane, tetrafluoro-	302–303
	+ sulfur fluoride, (OC-6-11)-	247–248
1-Nonanol	+ methane, tetrafluoro-	313
	+ sulfur fluoride, (OC-6-11)-	260–261
Nonene, octadecafluoro-	+ ethene, tetrafluoro-	406
Olive oil	+ methane, tetrafluoro-	332
	+ sulfur fluoride, (OC-6-11)-	289
Octane	+ methane, tetrafluoro-	302–305
	+ sulfur fluoride, (OC-6-11)-	247–249
1-Octanol	+ methane, tetrafluoro-	313, 316
	+ sulfur fluoride, (OC-6-11)-	233, 260–261, 264
Oxepane	+ methane, tetrafluoro-	322
	+ sulfur fluoride, (OC-6-11)-	272
Paraffin oil	+ methane, fluoro-	341
Pentadecane	+ methane, tetrafluoro-	302–303
	+ sulfur fluoride, (OC-6-11)-	247–248
Pentadecane, 2,6,10,14-tetramethyl-	+ ethane, 1,1-difluoro-	379
	+ ethane, pentafluoro-	349
	+ ethane, 1,1,1,2-tetrafluoro-	357
	+ ethane, 1,1,1-trifluoro-	373
Pentaerythritol tetra-2-ethylbutanoate	+ ethane, 1,1-difluoro-	384
	+ ethane, pentafluoro-	353
	+ ethane, 1,1,1,2-tetrafluoro-	362
	+ ethane, 1,1,1-trifluoro-	374
	+ methane, difluoro-	337
Pentaerythritol tetra-2-ethylhexanoate	+ ethane, 1,1-difluoro-	384
	+ ethane, pentafluoro-	354
	+ ethane, 1,1,1,2-tetrafluoro-	363
	+ ethane, 1,1,1-trifluoro-	375
	+ methane, difluoro-	336
Pentaerythritol tetrananoate ester	+ ethane, 1,1-difluoro-	385
	+ ethane, pentafluoro-	354
	+ ethane, 1,1,1,2-tetrafluoro-	363
	+ ethane, 1,1,1-trifluoro-	375
	+ methane, difluoro-	336
Pentaerythritol tetrapentanoate ester	+ ethane, 1,1-difluoro-	383

	+ ethane, pentafluoro-	353
	+ ethane, 1,1,1,2-tetrafluoro-	362
	+ ethane, 1,1,1-trifluoro-	374
	+ methane, difluoro-	335
Pentane	+ borane, trifluoro-	218
	+ sulfur fluoride, (OC-6-11)-	247
Pentane, 2,2,4-trimethyl-	+ methane, tetrafluoro-	304–305
	+ sulfur fluoride, (OC-6-11)-	250–251, 258
Pentane, 2,2,4-trimethyl- + benzene (mixture)	+ sulfur fluoride, (OC-6-11)-	258
2,4-Pentanediol, 2-methyl-	+ ethane, 1,1,1,2-tetrafluoro-	364
Pentanols mixture (amyl alcohol)	+ silane, tetrafluoro-	419–420
1-Pentanol	+ methane, tetrafluoro-	313
	+ sulfur fluoride, (OC-6-11)-	233, 260–261
Perfluoropropyl vinyl ether, see propane, 1,1,1,2,2,3,3-heptafluoro-3-(trifluoroethenyl)oxy-		
Perfluoropropene vinyl ether, see 1-propene, 1,1,2,3,3-pentafluoro-3-(trifluoroethenyl)oxy-		
Perfluorotribulyl amine, see 1-butanamine, 1,1,2,2,3,3,4,4,4-nonafluoro-*N*, *N*-*bis*(nonafluorrobutyl)-		
Phosphinic, diphenyl-, chloride	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
Phosphoric acid, hexamethyl, triamide	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
Phosphoric acid, tributyl ester	+ ethane, fluoro-	390
Phosphoric acid, triethyl ester	+ ethane, fluoro-	391
Phosphoric acid, trimethyl ester	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
Plasma, human	+ sulfur fluoride, (OC-6-11)-	288
Polyalkylene-glycol oil	+ ethane, 1,1,1,2-tetrafluoro-	368
Polyester mixture	+ ethane, 1,1,1,2-tetrafluoro-	369
Polyol ester mixture	+ ethane, pentafluoro-	355
	+ ethane, 1,1,1,2-tetrafluoro-	370
	+ methane, difluoro-	338
Potassium bromide (aqueous)	+ sulfur fluoride, (OC-6-11)-	E240–E241, 244
Potassium chloride (aqueous)	+ methan, tetrafluoro-	E298
	+ sulfur fluoride, (OC-6-11)-	E240–E241, 244
Potassium hydroxide (aqueous)	+ methane, tetrafluoro-	291
	+ sulfur fluoride, (OC-6-11)-	231, E240–E241
Potassium iodide (aqueous)	+ sulfur fluoride, (OC-6-11)-	E240–E241, 244
Propane, 1,1,1,2,2,3,3-heptafluoro-3-(trifluoroethenyl)-oxo-	+ ethene, tetrafluoro-	407
1,2,3-Propanetriol	+ silane, tetrafluoro-	419–420
1-Propene, 1,1,2,3,3-pentafluoro-3-(trifluoroethenyl)oxy-	+ ethene, tetrafluoro-	402
Propanoic acid, 2-oxo-(pyruvic acid)	+ silane, tetrafluoro-	419–420
1-Propanol	+ methane, fluoro-	342
	+ methane, tetrafluoro-	313–314
	+ sulfur fluoride, (OC-6-11)-	233, 260–261
1-Propanol, 2-methyl-	+ methane, tetrafluoro-	315
	+ sulfur fluoride, (OC-6-11)-	233, 262
2-Propanol	+ ethane, 1,1-difluoro-	382
	+ ethane, pentafluoro-	352
	+ ethane, 1,1,1,2-tetrafluoro-	360
	+ methane, difluoro-	335
	+ silane, tetrafluoro-	419–420
2-Propanol, 2-methyl-	+ sulfur fluoride, (OC-6-11)-	263
2-Propanol, 1,1,1,3,3,3-hexafluoro-	+ methane, tetrafluoro-	324
	+ sulfur fluoride, (OC-6-11)-	265
2-Propanol, 1,1,1,3,3,3-hexafluoro-(aqueous)	+ methane, tetrafluoro-	302
	+ sulfur fluoride, (OC-611)-	246
2-Propanone	+ ethane, 1,1-difluoro-	382
	+ ethane, fluoro-	386
	+ ethene, fluoro-	409–410
	+ silane, tetrafluoro-	419–420
	+ sulfur fluoride, (OC-6-11)-	266
Pyran, tetrahydro-2*H*-	+ methane, tetrafluoro-	322
	+ sulfur fluoride, (OC-6-11)-	270
Pyridine	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
2-Pyrrolidinone, 1-methyl-	+ cyclobutane, octafluoro-	399
	+ ethane, fluoro-	390
	+ ethene, fluoro-	412
	+ propene, hexafluoro-	415

Pyruvic acid, see propanoic acid, 2-oxo-	+ ethane, fluoro-	390
Quinoline		
Red cell ghosts, human, suspended in buffer	+ sulfur fluoride, (OC-6-11)-	286
Saline, normal	+ methane, difluoro-	332
	+ sulfur fluoride, (OC-6-11)-	236
Salt melt; $LiF+BeF_2$	+ borane, trifluoro-	224
Salt melt; $LiF+BeF_2+ThF_{4=}$	+ Borane, trifluoro-	224
Salt melt; $NaF+LiF+BeF_2+ThF_4$	+ borane, trifluoro-	224
Salt melt; $UF_4+ThF_4+BeF_2+LiF$	+ borane, trifluoro-	224
SDS, see sulfuric acid monododecyl ester sodium salt		
Seawater	+ methane, tetrafluoro-	297
	+ sulfur fluoride, (OC-6-11)-	238
Silane, tetrachloro-	+ sulfur fluoride, (OC-6-11)-	284
Silane, tetramethyl-	+ sulfur fluoride, (OC-6-11)-	284
Sodium chloride (aqueous)	+ ethane, 1,1-difluoro-	377
	+ ethane, 1,1,1,2-tetrafluoro-	356
	+ methane, tetrafluoro-	E298, 298
	+ methane, trifluoro-	E328, 330
	+ sulfur fluoride, (OC-6-11)-	E240–E241, 243
Sodium sulfate (aquous)	+ sulfur fluoride, (OC-6-11)-	E240–E241, 243
Sulfamide, tetraethyl-	+ methane, oxy*bis*(trifluoro)-	416
	+ propene, hexafluoro-	414
Sulfonamide, *N*,*N*-diethyl ethane-	+ methane, oxy*bis*trifluoro-	417
	+ propene, hexafluoro-	413
Sulfonamide, *N*,*N*-dimethyl ethane-	+ methane, oxy*bis*trifluoro-	416
	+ propene, hexafluoro-	414
Sulfonamide, *N*,*N*-diethyl methane-	+ methane, oxy*bis*trifluoro-	417
	+ propene, hexafluoro-	415
Sulfur dioxide, liquid	+ xenon fluoride, XeF_2 (qualitative observation)	E205–E206
Sulfuric acid	+ methane, tetrafluoro-	291
	+ borane, trifluoro-	223
Sulfuric acid monododecyl ester sodium salt (aqueous)	+ methane, tetrafluoro-	291, E298, 300
Superacid solvent; $HSO_3F+SbF_3+SO_3$	+ nitrogen fluoride, NF_3	227
Surface active agents (aqueous)	+ ethene, tetrafluoro-	402
Tetracosane	+ ethane, 1,1-difluoro-	
	+ methane, difluoro-	332
Tetradecane	+ methane, tetrafluoro-	302–303
	+ sulfur fluoride, (OC-6-11)-	247–248
Tetraethylammonium bromide, see 1-ethanaminium, *N*,*N*,*N*-triethyl bromide		
Tetraethylene glycol, see ethanol, 2,2′-[oxy*bis*(2,1-ethane-diyloxy)]*bis*-		
Tetraethylene glycol dimethyl ether	+ ethane, 1,1,1,2-tetrafluoro-	367
	+ ethane, 1,1,2,2-tetrafluoro-	371
	+ methane, tetrafluoro-	323
	+ sulfur fluoride, (OC-6-11)-	
Tetramethylammonium iodide, see methanaminium, *N*,*N*,*N*-trimethyl iodide		
Toluene, see benzene, methyl-		
Tridecane	+ ethane, 1,1,1,2-tetrafluoro-	356
	+ methane, tetrafluoro-	302–303
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