IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 2. Benzene with Water and Heavy Water

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The mutual solubilities and related liquid-liquid equilibria of benzene with water and heavy water are exhaustively and critically reviewed. Reports of experimental determination of solubility in these two chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For the system benzene-water sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of all experimental data for a homologous series of aromatic hydrocarbons was used. © *2005 American Institute of Physics.*
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Key words: benzene; critical evaluation; heavy water; liquid-liquid equilibria; solubilities; water

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1. Preface

1.1. Scope of this Volume

This paper is Part 2 of a revised and updated version of an earlier compilation and evaluation of the mutual solubilities of water and hydrocarbon compounds containing five or more carbon atoms.[1,2] This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) together with new compilations based on recent and previously overlooked reports in the peer-reviewed scientific literature prior to 2003. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators.

This revised work includes a new critical evaluation in which reported solubility values are characterized as recommended, tentative, doubtful, or rejected. This classification is based on the consistency between independently determined experimental values and reference values derived from a newly developed set of smoothing equations.[3] Recommended values are supported by two (or more) independent experimental values and a reference value that are all in agreement. Tentative values are supported by two (or more) independent values in agreement with each other, but not with the reference value, or one experimental value in agreement with the reference value. Doubtful values are those for which a single experimental value differs from the reference value. Experimental values that differ from reference values and other experimental values or experimental values that were obtained by suspect or undefined methods are rejected.

Detailed introductory material including explanations of the formats of compilation, definitions of commonly used measures of solubility, the derivation of the smoothing equations used calculate reference values, and the scope of the Solubility Data Series can be found in Part 1 of this updated series.[4]

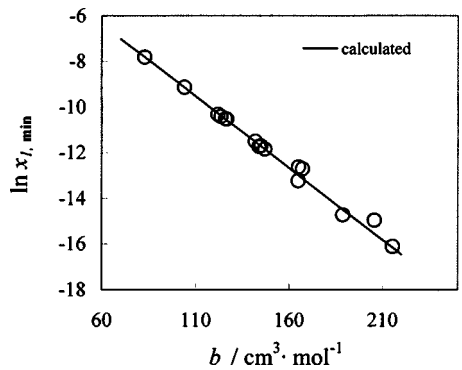

FIG. 1. Minimum solubilities ($x_{1,\min}$) of aromatic hydrocarbons vs excluded volume (b).

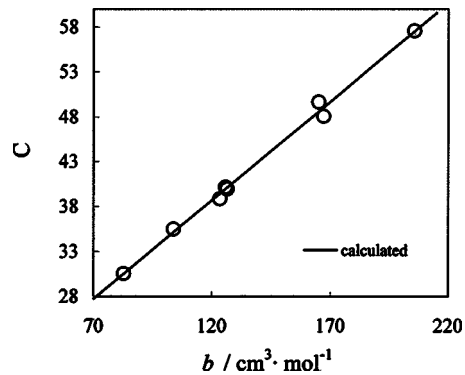

FIG. 2. Coefficient C vs excluded volume of aromatic hydrocarbons (b).

1.2. Procedures Used in Critical Evaluation

The procedures used in critical evaluation and derivation of reference data for systems containing aromatic hydrocarbons and water[3] are similar to those used for aliphatic hydrocarbons and water.[4–7]

Derivation of Reference Data for Solubility of Aromatic Hydrocarbons in Water

The mole fraction of aromatic hydrocarbons in water (x_1) at temperature (T) along the three phase equilibrium exhibits a minimum ($x_{1,\min}$) near room temperature $T_{\min}$. The solubility curve can be calculated approximately with an earlier derived equation:[3]

$$\ln x_1 = \ln x_{1,\min} + \mathrm{C} f(T/T_{\min}) \tag{1}$$

where C is an adjustable parameter dependent on hydrocarbons and $f(T/T_{\min})$ is a function, which achieves minimum value equal to zero at $T = T_{\min}$:

$$f(T/T_{\min}) = [(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)]. \tag{2}$$

Equation (1) was fitted to experimental solubility curves reported in the literature for various aromatic hydrocarbons. The fitted values of $T_{\min}$ are sensitive to errors of the data. Taking into account the obtained, randomly scattered values was decided to use $T_{\min} = 290$ K for all investigated systems.

The other two parameters ($x_{1,\min}$ and C) are related to volume of the hydrocarbon. Larger molecules exhibit lower solubility, because the number of hydrogen bonds broken and distorted during solution depends very much on the size of the cavity in the water needed to accommodate the dissolved molecule. It is assumed here that the size of the cavity is proportional to the excluded volume (b) of the hydrocarbon. In this work *Redlich–Kwong* Equation of State (RK EoS) is used, where b is calculated from the critical temperature (T_c) and critical pressure (P_c).

$$b = 0.08664 \ \mathrm{R} T_c / P_c. \tag{3}$$

The adjusted values of $\ln x_{1,\min}$ and C are plotted vs b in Figs. 1 and 2.

The linear relations shown in Figs. 1 and 2 suggest that Eq. (1) can be rewritten in form

$$\ln x_1 = (c_1 + c_2 b) + (c_3 + c_4 b) f(T/T_{\min}). \tag{4}$$

The coefficients c_1, c_2, c_3, and c_4 were found by simultaneous regression of the investigated solubility data. Before regression the plots of the solubility data were inspected in order to remove outlying experimental points. The initial verification rejected 210 points. The remaining 556 points corresponding to 24 mixtures were used in the regression. The following values of the coefficient in Eq. (4) were obtained:

$$c_1 = -2.605; \quad c_2 = -0.06296 \ \mathrm{cm}^{-3}\mathrm{mol};$$

$$c_3 = 7.979; \quad c_4 = 0.2668 \ \mathrm{cm}^{-3}\mathrm{mol}.$$

These values applied to benzene ($b = 82.7$ cm^3 mol^{-1}) give:

$$\ln x_1 = -7.812 + 30.04 f(T/T_{\min}). \tag{5}$$

Equation (4) with the obtained coefficients is valid up to three phase critical temperature (T_{3c}). The solubility of benzene in water reported for temperatures higher than T_{3c} are also well approximated. The analysis of the deviations for the investigated systems shows that they are random and can be ascribed to error of the data.

The standard error of $\ln(x_1)$ resulting from Eq. (4) was determined with help of the variance–covariance matrix obtained by the least squares method. For benzene this yields the following equation:

$$s(\ln x_1) = [1.83\times 10^{-4} - 2.45\times 10^{-3} f(T/T_{\min}) + 0.202 f^2(T/T_{\min})]^{0.5}, \tag{6}$$

where $f(T/T_{\min})$ is defined with Eq. (2). The value of $s(\ln x_1)$, calculated with Eq. (6), is 0.014 at 290 K and increases with temperature achieving 0.057 at 550 K.

The solubility of hydrocarbons in water calculated from Eq. (4) are used as reference data. It was assumed that the error of the reference data does not exceed three times the

standard deviation. As in Part 1 (Maczynski and Shaw[4]), experimental solubility differing from the reference data more than the 30% are considered doubtful. Data are regarded as tentative if they agree with the reference data but are not supported by measurements from other laboratories. Data from different sources, which agree with each other and with the reference data are recommended.

Derivation of Reference Data for Solubility of Water in Aromatic Hydrocarbons

Reference data for the solubility of water in aromatic hydrocarbons were calculated by a method developed by Góral.[8] This method of phase equilibrium calculations (EoSC) is based on the RK EoS with an added term, which accounts for hydrogen bonding. Application of the EoSC for water systems has been described earlier.[4–7] The input data for the LLE correlation in aromatic hydrocarbon–water systems is the solubility of the aromatic hydrocarbons in water, calculated with Eq. (4). The output is water solubility (x_2) in a given hydrocarbon as a function of temperature (T).

The calculated results were compared with experimental data[3] and support the conclusion that the calculated solubilities of water in aromatic hydrocarbons can be used as reference data up to about 60 K below the three phase temperature.

Standard error of the water solubility measurements was estimated with equation:

$$s(\ln x_{2,\mathrm{exp}})=[\Sigma(\ln x_{2,\mathrm{exp}}-\ln x_{2,\mathrm{EoSC}})_k/(m-n)]^{0.5}, \tag{7}$$

where $\ln x_{2,\mathrm{exp}}$ is a logarithm of the experimental mole fraction of water in hydrocarbon and $\ln x_{2,\mathrm{EoSC}}$ is the corresponding value calculated with EoSC using n parameters in the model of the association. The summation goes through m experimental points.

For the solubility of water in the aromatic hydrocarbons 405 experimental points for 15 systems were available in the literature. Most of these points (270) correspond to solubility of water in benzene or toluene. After initial verification 36 points were rejected. Standard error estimated from the remained 369 points was 0.11. In view of accuracy of the data the agreement between the calculated and experimental water solubilities is very satisfactory.

Average standard errors of the calculated (reference) data was estimated with equation:

$$\overline{s}(\ln x_{2,\mathrm{EoSC}})=s(\ln x_{2,\mathrm{exp}})(n/m)^{0.5}, \tag{8}$$

where $m=369$; $n=3$; $s(\ln x_{2,\mathrm{exp}})=0.11$, which gives: $\overline{s}(\ln x_{2,\mathrm{EoSC}})=0.01$. This corresponds to an average standard error of the calculated mole fraction of water about 1%. One must take into account that Eq. (8) gives an average value of the standard error. This error is certainly larger at high temperatures, because most of the experimental points are reported for low and medium temperatures. This situation is similar to those presented in the previous section, where Eq. (6) gives standard error equal about 0.01 at low temperatures and 0.06 at high temperature. Therefore we used the same criteria as those adopted in previous section for recommended, tentative, and doubtful data.

For convenience of the user the solubility of water in benzene predicted with EoSC were approximated with Eq. (9) proposed by Economou *et al.*[9]

$$\ln x_2=d_1+d_2(1/T_r-1)+d_3(1-T_r)^{1/3}+d_4(1-T_r), \tag{9}$$

where $T_r=T/T_{3c}$, and T_{3c} is three phase critical temperature. According to Tsonopoulos and Wilson[10] for benzene $T_{3c}=541.7$ K. Values of the coefficients adjusted to the solubility data predicted by EoSC are as follows: $d_1=-0.509$; $d_2=-4.316$; $d_3=-0.203$; $d_4=-3.637$.

The range of applicability of Eq. (9) is the same as those listed above for EoSC.

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1.3. References for the Preface

[1] D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 37, Hydrocarbons with Water and Seawater, Part I: *Hydrocarbons C5 to C7* (Pergamon Press, New York, 1989).
[2] D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 38, Hydrocarbons with Water and Seawater, Part II: *Hydrocarbons C8 to C36* (Pergamon Press, New York, 1989).
[3] B. Wisniewska-Goclowska, A. Maczynski, and M. Goral, Recommended Liquid-Liquid Equilibrium Data, Part 3: Binary Aromatic Hydrocarbons-Water Systems, J. Phys. Phys. Chem. Ref. Data (submitted).
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[10] C. Tsonopoulos and G. M. Wilson, AIChEJ. **29**, 990 (1983).

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

2.1. Nature of the Project

The Solubility Data project 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.

This series is concerned primarily with liquid-liquid systems, but a limited number or related solid-liquid, fluid-fluid, and multicomponent (organic-water-salt) systems are included where it is considered logical and appropriate. Solubilities at elevated and low temperatures and at elevated pressures have also been included, as it is considered inappropriate to establish artificial limits on the data presented if they are considered relevant or useful.

For some systems, the two components may be miscible in all proportions at certain temperatures and pressures. Data on reported miscibility gaps and upper and lower critical solution temperatures are included where appropriate and when available.

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 previous *Solubility Data Series* volumes, for example, Sazonov and Shaw.[1]

Solubilities of liquids in liquids and solids 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 Sazonov and Shaw.[1] A few quantities follow the ISO standards[3] or the German standard;[4] see a review by Cvitaš[5] for details. 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 by Lorimer.[6]

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

[1] V. P. Sazonov and D. G. Shaw, editors, *Acetonitrile Binary Systems*, IUPAC-NIST Solubility Data Series, Vol. 79, J. Phys. Chem. Ref. Data **31** (4), 989 (2002).

[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).

[4] German Standard, DIN 1310, *Zusammungsetzung von Mischphasen* (Beuth Verlag, Berlin, 1984).

[5] T. Cvitaš, Chem. International **17** (4), 123 (1995).

[6] J. W. Lorimer, *Quantities, Units and Conversions*, in *The Experimental Determination of Solubilities*, G. T. Hefter and R. P. T. Tomkins, editors (Wiley, New York, 2003).

3. Benzene with Water and Heavy Water

3.1. Benzene with Water

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland September, 2003

Critical Evaluation of the Solubility of Benzene (1) in Water (2)

Experimental solubility data for (1) in (2) have been reported in the 66 publications listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Alexander[1]	274–339	Korenman and Arefeva[55]	298
Anderson and Prausnitz[3]	374–477 (287–3218 kPa)	Krasnoshchekova and Gubergrits[56]	298
Andrews and Keefer[4]	298	Leinonen and Mackay[58]	298
Arnold *et al.*[5]	279–342	Lo *et al.*[59]	298
Banerjee *et al.*[6]	298	Mackay and Shiu[60]	298
Barbaudy[7]	342	May *et al.*[62]	298
Ben-Naim and Wilf[9]	283–293	May *et al.*[63]	273–299
Ben-Naim and Wilf[10]	298	McAuliffe[64]	298
Bittrich *et al.*[12]	293–333	McBain and Lissant[65]	298
Bohon and Claussen[14]	298	McCants *et al.*[66]	311
Booth and Everson[15]	298	McDevit and Long[67]	298
Booth and Everson[16]	298–333	Miller and Hawthorne[68]	298–473 (100–6500 kPa)
Bradley *et al.*[17]	298–328	Milligan[69]	298
Brady and Huff[18]	298	Morrison and Billett[70]	298
Brown and Wasik[19]	278–293	Niini[72]	293
Budantseva *et al.*[20]	293	Pierotti and Liabastre[75]	278–319
Chandler *et al.*[23]	473–548 (2700–6600)	Polak and Lu[76]	273–298
Chen and Wagner[24]	303–373 (100–350 kPa)	Price[77]	298
Chey and Calder[25]	294	Sada *et al.*[82]	298
Corby and Elworthy[28]	293	Sanemasa *et al.*[83]	298
Donahue and Bartell[29]	298	Sanemasa *et al.*[84]	278–318
Durand[30]	289	Sanemasa *et al.*[85]	288–318
Franks *et al.*[33]	290–336	Sanemasa *et al.*[86]	298
Gramajo de Doz *et al.*[35]	303	Saylor *et al.*[88]	303–308
Griswold *et al.*[37]	298–323	Schwarz[90]	297
Gross and Saylor[39]	303	Stearns *et al.*[95]	298
Guseva and Parnov[40]	426–527	Stephenson[96]	298
Hayashi and Sasaki[41]	293–298	Taha *et al.*[97]	298
Herz[42]	295	Tsonopoulos and Wilson[100]	313–473 (30–3020 kPa)
Hill[43]	273	Udovenko and Aleksandrova[101]	293–353
Janado *et al.*[47]	298	Uspenskii[102]	283–295
Keeley *et al.*[51]	298	Vesala[103]	298
Klevens[53]	275	Worley[105]	298
Korenman and Aref'eva[54]	293		

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface and expressed by Eq. (1)

$$\ln x_1 = \ln x_{\min,1} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where: $\ln x_{\min,1} = -7.812$; $D = 30.04$; $T_{\min} = 290$.

In contrast to the smoothed equation used by Hefter and Young[125] for regression of the solubility data of benzene in water, Eq. (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in the Table 1.

All the experimental and reference data are listed in Table 2 and shown in Fig. 3.The recommended and tentative data are shown in Fig. 4.

TABLE 1. The data categories for solubility of benzene (1) in water (2)

T/K	Recommended (data in good agreement with each other and with the reference data)	Tentative (data in good agreement with the reference data)	Doubtful (data in poor agreement with the reference data)
273.1	Hill[43]		
	Polak and Lu[76]		
273.4		May *et al.*[63]	
274.0		Alexander[1]	
275.2		Klevens[53]	
277.7		Brown and Wasik[19]	
278.2		Pierotti and Liabastre[75]	
		Sanemasa *et al.*[84]	
278.8		Arnold *et al.*[5]	
279.4		May *et al.*[63]	
279.5		Brown and Wasik[19]	
279.9		Arnold *et al.*[5]	
280.3		Brown and Wasik[19]	
282.2	Arnold *et al.*[5]		
	Brown and Wasik[19]		
282.6		Alexander[1]	
283.2	Ben-Naim and Wilf[9]		
	Uspenskii[102]		
284.4		May *et al.*[63]	
285.0		Brown and Wasik[19]	
285.3		Brown and Wasik[19]	
285.7		Arnold *et al.*[5]	
287.2		May *et al.*[63]	
288.1		Pierotti and Liabastre[75]	
288.2	Arnold *et al.*[5]		
	Sanemasa *et al.*[84]		
	Sanemasa *et al.*[85]		
288.3		Brown and Wasik[19]	
289.2		Durand[30]	
290.0		Alexander[1]	
290.1		May *et al.*[63]	
290.2		Franks *et al.*[33]	
291.1		Brown and Wasik[19]	
291.8		May *et al.*[63]	
293.1		Pierotti and Liabastre[75]	
293.2	Arnold *et al.*[5]	Hayashi and Sasaki[41]	Korenman and Aref'eva[54]
	Ben-Naim and Wilf[9]	Udovenko and Aleksandrova[101]	Niini[72]
	Bittrich *et al.*[12]		
	Budantseva *et al.*[20]		
	Corby and Elworthy[28]		

293.3		Brown and Wasik[19]	
293.8		Arnold *et al.*[5]	
294.0		Chey and Calder[25]	
295.2		Franks *et al.*[33]	Herz[42]
		Uspenskii[102]	
296.7		Schwarz[90]	
297.2		Alexander[1]	
298.0	Arnold *et al.*[5]	Miller and Hawthorne[68]	
	Miller and Hawthorne[68]	Vesala[103]	
298.1		Arnold *et al.*[5]	
		Sanemasa *et al.*[86]	
298.2	Andrews and Keefer[4]	Booth and Everson[15]	Booth and Everson[16]
	Banerjee *et al.*[6]	McBain and Lissant[65]	Korenman and Aref'eva[55]
	Ben-Naim and Wilf[10]	Sanemasa *et al.*[83]	Krasnoshchekova and
	Bohon and Claussen[14]	Sanemasa *et al.*[84]	Gubergrits[56]
	Bradley *et al.*[17]	Sanemasa *et al.*[85]	Milligan[69]
	Brady and Huff[18]	Stephenson[96]	Stearns *et al.*[95]
	Donahue and Bartell[29]	Worley[105]	
	Griswold *et al.*[37]		
	Hayashi and Sasaki[41]		
	Janado *et al.*[47]		
	Keeley *et al.*[51]		
	Leinonen and Mackay[58]		
	Lo *et al.*[59]		
	Mackay and Shiu[60]		
	May *et al.*[62]		
	May *et al.*[63]		
	McAuliffe[64]		
	McDevit and Long[67]		
	Morrison and Billett[70]		
	Pierotti and Liabastre[75]		
	Polak and Lu[76]		
	Price[77]		
	Sada *et al.*[82]		
	Taha *et al.*[97]		
299.0		May *et al.*[63]	
299.2		Franks *et al.*[33]	
300.5		Arnold *et al.*[5]	
302.2		Franks *et al.*[33]	
303.2	Arnold *et al.*[5]	Gramajo de Doz *et al.*[35]	
	Chen and Wagner[24]	Udovenko and	
	Gross and Saylor[39]	Aleksandrova[101]	
	Saylor *et al.*[88]		
304.2		Alexander[1]	
305.2		Franks *et al.*[33]	
308.2	Arnold *et al.*[5]	Sanemasa *et al.*[84]	
	Franks *et al.*[33]		
	Sanemasa *et al.*[85]		
	Saylor *et al.*[88]		
308.3		Pierotti and Liabastre[75]	
311.0			McCants *et al.*[66]

311.2		Alexander[1]	
313.1		Arnold *et al.*[5]	
313.2	Bittrich *et al.*[12]		
	Chen and Wagner[24]		
	Tsonopoulos and		
	Wilson[100]		
313.7		Franks *et al.*[33]	
		Udovenko and	
		Aleksandrova[101]	
315.2		Franks *et al.*[33]	
317.2		Franks *et al.*[33]	
317.7			Udovenko and
			Aleksandrova[101]
317.9		Alexander[1]	
318.2	Arnold *et al.*[5]	Bradley *et al.*[17]	
	Bradley *et al.*[17]	Sanemasa *et al.*[84]	
		Sanemasa *et al.*[85]	
318.9		Pierotti and Liabastre[75]	
319.2		Franks *et al.*[33]	
323.0	Arnold *et al.*[5]		
	Miller and Hawthorne[68]		
323.2	Chen and Wagner[24]		
	Griswold *et al.*[37]		
324.2		Franks *et al.*[33]	
324.7		Alexander[1]	
327.7		Arnold *et al.*[5]	
328.2		Bradley *et al.*[17]	
329.2		Franks *et al.*[33]	
329.7			Udovenko and
			Aleksandrova[101]
332.0		Alexander[1]	
333.0		Arnold *et al.*[5]	
333.2	Bittrich *et al.*[12]	Booth and Everson[16]	Udovenko and
	Chen and Wagner[24]		Aleksandrova[101]
334.2		Franks *et al.*[33]	
336.2		Franks *et al.*[33]	
338.0		Arnold *et al.*[5]	
338.2			Udovenko and
			Aleksandrova[101]
338.6		Alexander[1]	
342.2		Arnold *et al.*[5]	
342.4		Barbaudy[7]	
343.2		Chen and Wagner[24]	
352.7		Udovenko and	
		Aleksandrova[101]	
353.2		Chen and Wagner[24]	
363.2		Chen and Wagner[24]	
373.0		Miller and Hawthorne[68]	
373.2	Chen and Wagner[24]		
	Tsonopoulos and		
	Wilson[100]		

374.2		Anderson and Prausnitz[3]	
398.0		Anderson and Prausnitz[3]	
420.9		Anderson and Prausnitz[3]	
423.0	Anderson and Prausnitz[3] Miller and Hawthorne[68]		
423.2		Tsonopoulos and Wilson[100]	
426.2			Guseva and Parnov[40]
448.0		Anderson and Prausnitz[3]	
448.6		Anderson and Prausnitz[3]	
451.2			Guseva and Parnov[40]
473.0		Miller and Hawthorne[68]	
473.2		Chandler *et al.*[23] Tsonopoulos and Wilson[100]	
473.4		Anderson and Prausnitz[3]	
477.0		Anderson and Prausnitz[3]	
477.2		Guseva and Parnov[40]	
498.2	Chandler *et al.*[23] Guseva and Parnov[40]		
514.2		Guseva and Parnov[40]	
523.2		Chandler *et al.*[23]	
527.2		Guseva and Parnov[40]	

TABLE 2. Experimental values for solubility of benzene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2		$3.53\cdot10^{-4}$ (R; Ref. 43), $3.87\cdot10^{-4}$ (R; Ref. 76)	$4.3\cdot10^{-4}$
273.4		$4.232\cdot10^{-4}$ (T; Ref. 63)	$4.3\cdot10^{-4}$
274.0		$4.25\cdot10^{-4}$ (T; Ref. 1)	$4.3\cdot10^{-4}$
275.2		$4.31\cdot10^{-4}$ (T; Ref. 53)	$4.2\cdot10^{-4}$
277.7		$4.25\cdot10^{-4}$ (T; Ref. 19)	$4.2\cdot10^{-4}$
278.2		$4.776\cdot10^{-4}$ (T; Ref. 75), $3.73\cdot10^{-4}$ (T; Ref. 84)	$4.2\cdot10^{-4}$
278.8		$4.02\cdot10^{-4}$ (T; Ref. 5)	$4.2\cdot10^{-4}$
279.4		$4.159\cdot10^{-4}$ (T; Ref. 63)	$4.1\cdot10^{-4}$
279.5		$4.27\cdot10^{-4}$ (T; Ref. 19)	$4.1\cdot10^{-4}$
279.9		$4.02\cdot10^{-4}$ (T; Ref. 5)	$4.1\cdot10^{-4}$
280.3		$4.18\cdot10^{-4}$ (T; Ref. 19)	$4.1\cdot10^{-4}$
282.2		$3.99\cdot10^{-4}$ (R; Ref. 5), $4.18\cdot10^{-4}$ (R; Ref. 19)	$4.1\cdot10^{-4}$
282.6		$4.13\cdot10^{-4}$ (T; Ref. 1)	$4.1\cdot10^{-4}$
283.2		$3.75\cdot10^{-4}$ (R; Ref. 9), $4.04\cdot10^{-4}$ (R; Ref. 102)	$4.1\cdot10^{-4}$
284.4		$4.147\cdot10^{-4}$ (T; Ref. 63)	$4.1\cdot10^{-4}$
285.0		$4.09\cdot10^{-4}$ (T; Ref. 19)	$4.1\cdot10^{-4}$
285.3		$4.09\cdot10^{-4}$ (T; Ref. 19)	$4.1\cdot10^{-4}$
285.7		$3.97\cdot10^{-4}$ (T; Ref. 5)	$4.1\cdot10^{-4}$
287.2		$4.08\cdot10^{-4}$ (T; Ref. 63)	$4.1\cdot10^{-4}$
288.1		$4.792\cdot10^{-4}$ (T; Ref. 75)	$4.1\cdot10^{-4}$
288.2		$3.99\cdot10^{-4}$ (R; Ref. 5), $3.65\cdot10^{-4}$ (R; Ref. 84), $3.56\cdot10^{-4}$ (R; Ref. 85)	$4.1\cdot10^{-4}$
288.3		$4.14\cdot10^{-4}$ (T; Ref. 19)	$4.1\cdot10^{-4}$
289.2		$3.35\cdot10^{-4}$ (T; Ref. 30)	$4.1\cdot10^{-4}$
290.0		$4.09\cdot10^{-4}$ (T; Ref. 1)	$4.1\cdot10^{-4}$
290.1		$4.062\cdot10^{-4}$ (T; Ref. 63)	$4.1\cdot10^{-4}$
290.2		$3.95\cdot10^{-4}$ (T; Ref. 33)	$4.1\cdot10^{-4}$
291.1		$4.14\cdot10^{-4}$ (T; Ref. 19)	$4.1\cdot10^{-4}$
291.8		$4.073\cdot10^{-4}$ (T; Ref. 63)	$4.1\cdot10^{-4}$
293.1		$4.809\cdot10^{-4}$ (T; Ref. 75)	$4.1\cdot10^{-4}$
293.2		$3.95\cdot10^{-4}$ (R; Ref. 5), $4.01\cdot10^{-4}$ (R; Ref. 9), $4.133\cdot10^{-4}$ (R; Ref. 12), $4.00\cdot10^{-4}$ (R; Ref. 20), $3.90\cdot10^{-4}$ (R; Ref. 28), $3.16\cdot10^{-4}$ (T; Ref. 41), $1.94\cdot10^{-4}$ (D; Ref. 54), $2.00\cdot10^{-4}$ (D; Ref. 72), $4.85\cdot10^{-4}$ (T; Ref. 101)	$4.1\cdot10^{-4}$
293.3		$4.07\cdot10^{-4}$ (T; Ref. 19)	$4.1\cdot10^{-4}$
293.8		$3.97\cdot10^{-4}$ (T; Ref. 5)	$4.1\cdot10^{-4}$
294.0		$4.01\cdot10^{-4}$ (T; Ref. 25)	$4.1\cdot10^{-4}$
295.2		$3.97\cdot10^{-4}$ (T; Ref. 33), $1.67\cdot10^{-4}$ (D; Ref. 42), $4.306\cdot10^{-4}$ (T; Ref. 102)	$4.1\cdot10^{-4}$
296.7		$4.34\cdot10^{-4}$ (T; Ref. 90), $4.20\cdot10^{-4}$ (T; Ref. 90), $4.45\cdot10^{-4}$ (T; Ref. 90), $4.38\cdot10^{-4}$ (T; Ref. 90)	$4.1\cdot10^{-4}$
297.2		$4.16\cdot10^{-4}$ (T; Ref. 1)	$4.1\cdot10^{-4}$
298.0	100 (Ref. 68) 6500 (Ref. 68)	$3.95\cdot10^{-4}$ (R; Ref. 5), $4.00\cdot10^{-4}$ (R; Ref. 68), $4.00\cdot10^{-4}$ (R; Ref. 68), $4.40\cdot10^{-4}$ (T; Ref. 103)	$4.1\cdot10^{-4}$
298.1		$4.02\cdot10^{-4}$ (T; Ref. 5), $3.74\cdot10^{-4}$ (T; Ref. 86)	$4.1\cdot10^{-4}$
298.2	100 (Ref. 17)	$4.02\cdot10^{-4}$ (R; Ref. 4), $4.05\cdot10^{-4}$ (R; Ref. 6), $4.21\cdot10^{-4}$ (R; Ref. 10), $4.13\cdot10^{-4}$ (R; Ref. 14), $3.30\cdot10^{-4}$ (T; Ref. 15), $2.20\cdot10^{-4}$ (D; Ref. 16), $4.21\cdot10^{-4}$ (R; Ref. 17), $4.06\cdot10^{-4}$ (R; Ref. 18), $4.20\cdot10^{-4}$ (R; Ref. 29), $4.20\cdot10^{-4}$ (R; Ref. 37), $4.16\cdot10^{-4}$ (R; Ref. 41), $4.187\cdot10^{-4}$ (R; Ref. 47), $3.91\cdot10^{-4}$ (R; Ref. 51), $1.94\cdot10^{-4}$ (D; Ref. 55), $2.305\cdot10^{-4}$ (D; Ref. 56), $4.07\cdot10^{-4}$ (R; Ref. 58), $4.18\cdot10^{-4}$ (R; Ref. 59), $4.11\cdot10^{-4}$ (R; Ref. 60), $4.13\cdot10^{-4}$ (R; Ref. 62), $4.129\cdot10^{-4}$ (R; Ref. 63), $4.11\cdot10^{-4}$ (R; Ref. 64), $3.48\cdot10^{-4}$ (T; Ref. 65), $4.091\cdot10^{-4}$ (R; Ref. 67), $1.42\cdot10^{-4}$ (D; Ref. 69), $3.96\cdot10^{-4}$ (R; Ref. 70), $4.815\cdot10^{-4}$ (R; Ref. 75), $4.05\cdot10^{-4}$ (R; Ref. 76), $4.01\cdot10^{-4}$ (R; Ref. 77), $4.15\cdot10^{-4}$ (R; Ref. 82), $3.73\cdot10^{-4}$ (T; Ref. 83), $3.74\cdot10^{-4}$ (T; Ref. 84), $3.72\cdot10^{-4}$ (T; Ref. 85), $2.00\cdot10^{-4}$ (D; Ref. 95), $3.63\cdot10^{-4}$ (T; Ref. 96), $3.65\cdot10^{-4}$ (T; Ref. 96), $4.00\cdot10^{-4}$ (R; Ref. 97), $5.01\cdot10^{-4}$ (T; Ref. 105)	$4.1\cdot10^{-4}$
299.0		$4.193\cdot10^{-4}$ (T; Ref. 63)	$4.1\cdot10^{-4}$
299.2		$3.99\cdot10^{-4}$ (T; Ref. 33)	$4.1\cdot10^{-4}$
300.5		$4.02\cdot10^{-4}$ (T; Ref. 5)	$4.1\cdot10^{-4}$
302.2		$4.02\cdot10^{-4}$ (T; Ref. 33)	$4.2\cdot10^{-4}$

303.2	100 (Ref. 24)	$4.09\cdot10^{-4}$ (R; Ref. 5), $4.06\cdot10^{-4}$ (R; Ref. 5), $4.24\cdot10^{-4}$ (R; Ref. 24), $5.00\cdot10^{-4}$ (T; Ref. 35), $4.27\cdot10^{-4}$ (R; Ref. 39), $4.25\cdot10^{-4}$ (R; Ref. 88), $5.24\cdot10^{-4}$ (T; Ref. 101)	$4.2\cdot10^{-4}$
304.2		$4.23\cdot10^{-4}$ (T; Ref. 1)	$4.2\cdot10^{-4}$
305.2		$4.12\cdot10^{-4}$ (T; Ref. 33)	$4.2\cdot10^{-4}$
308.2		$4.20\cdot10^{-4}$ (R; Ref. 5), $4.20\cdot10^{-4}$ (R; Ref. 33), $3.94\cdot10^{-4}$ (T; Ref. 84), $4.09\cdot10^{-4}$ (R; Ref. 85), $4.38\cdot10^{-4}$ (R; Ref. 88)	$4.3\cdot10^{-4}$
308.3		$4.848\cdot10^{-4}$ (T; Ref. 75)	$4.3\cdot10^{-4}$
311.0		$1.20\cdot10^{-3}$ (D; Ref. 66)	$4.3\cdot10^{-3}$
311.2		$4.50\cdot10^{-4}$ (T; Ref. 1)	$4.3\cdot10^{-4}$
313.1		$4.34\cdot10^{-4}$ (T; Ref. 5)	$4.4\cdot10^{-4}$
313.2	100 (Ref. 24) 30.54 (Ref. 100)	$4.676\cdot10^{-4}$ (R; Ref. 12), $4.64\cdot10^{-4}$ (R; Ref. 24), $4.435\cdot10^{-4}$ (R; Ref. 100)	$4.4\cdot10^{-4}$
313.7		$4.39\cdot10^{-4}$ (T; Ref. 33), $5.73\cdot10^{-4}$ (T; Ref. 101)	$4.4\cdot10^{-4}$
315.2		$4.40\cdot10^{-4}$ (T; Ref. 33)	$4.5\cdot10^{-4}$
317.2		$4.45\cdot10^{-4}$ (T; Ref. 33)	$4.5\cdot10^{-4}$
317.7		$5.98\cdot10^{-4}$ (D; Ref. 101)	$4.6\cdot10^{-4}$
317.9		$4.69\cdot10^{-4}$ (T; Ref. 1)	$4.6\cdot10^{-4}$
318.2	100 (Ref. 17)	$4.55\cdot10^{-4}$ (R; Ref. 5), $4.53\cdot10^{-4}$ (R; Ref. 5), $4.99\cdot10^{-4}$ (T; Ref. 17), $4.15\cdot10^{-4}$ (T; Ref. 84), $4.32\cdot10^{-4}$ (T; Ref. 85)	$4.6\cdot10^{-4}$
318.9		$5.304\cdot10^{-4}$ (T; Ref. 75)	$4.6\cdot10^{-4}$
319.2		$4.57\cdot10^{-4}$ (T; Ref. 33)	$4.6\cdot10^{-4}$
323.0	6500 (Ref. 68)	$4.71\cdot10^{-4}$ (R; Ref. 5), $4.70\cdot10^{-4}$ (R; Ref. 68)	$4.8\cdot10^{-4}$
323.2	100 (Ref. 24)	$5.10\cdot10^{-4}$ (R; Ref. 24), $5.50\cdot10^{-4}$ (R; Ref. 37)	$4.8\cdot10^{-4}$
324.2		$4.78\cdot10^{-4}$ (T; Ref. 33)	$4.8\cdot10^{-4}$
324.7		$4.94\cdot10^{-4}$ (T; Ref. 1)	$4.8\cdot10^{-4}$
327.7		$4.97\cdot10^{-4}$ (T; Ref. 5)	$5.0\cdot10^{-4}$
328.2	100 (Ref. 17)	$5.49\cdot10^{-4}$ (T; Ref. 17)	$5.0\cdot10^{-4}$
329.2		$5.03\cdot10^{-4}$ (T; Ref. 33)	$5.1\cdot10^{-4}$
329.7		$6.65\cdot10^{-4}$ (D; Ref. 101)	$5.1\cdot10^{-4}$
332.0		$5.40\cdot10^{-4}$ (T; Ref. 1)	$5.2\cdot10^{-4}$
333.0		$5.22\cdot10^{-4}$ (T; Ref. 5)	$5.3\cdot10^{-4}$
333.2	150 (Ref. 24)	$5.641\cdot10^{-4}$ (R; Ref. 12), $3.90\cdot10^{-4}$ (T; Ref. 16), $5.65\cdot10^{-4}$ (R; Ref. 24), $6.93\cdot10^{-4}$ (D; Ref. 101)	$5.3\cdot10^{-4}$
334.2		$5.31\cdot10^{-4}$ (T; Ref. 33)	$5.3\cdot10^{-4}$
336.2		$5.42\cdot10^{-4}$ (T; Ref. 33)	$5.5\cdot10^{-4}$
338.0		$5.57\cdot10^{-4}$ (T; Ref. 5)	$5.6\cdot10^{-4}$
338.2		$7.37\cdot10^{-4}$ (D; Ref. 101)	$5.6\cdot10^{-4}$
338.6		$5.94\cdot10^{-4}$ (T; Ref. 1)	$5.6\cdot10^{-4}$
342.2		$5.67\cdot10^{-4}$ (T; Ref. 5)	$5.9\cdot10^{-4}$
342.4		$6.49\cdot10^{-4}$ (T; Ref. 7)	$5.9\cdot10^{-4}$
343.2	250 (Ref. 24)	$6.25\cdot10^{-4}$ (T; Ref. 24)	$5.9\cdot10^{-4}$
352.7		$8.62\cdot10^{-4}$ (T; Ref. 101)	$6.7\cdot10^{-4}$
353.2	250 (Ref. 24)	$6.99\cdot10^{-4}$ (T; Ref. 24)	$6.8\cdot10^{-4}$
363.2	350 (Ref. 24)	$8.00\cdot10^{-4}$ (T; Ref. 24)	$7.8\cdot10^{-4}$
373.0	6500 (Ref. 68)	$8.90\cdot10^{-4}$ (T; Ref. 68)	$9.1\cdot10^{-4}$
373.2	350 (Ref. 24) 275.8 (Ref. 100)	$9.50\cdot10^{-4}$ (R; Ref. 24), $9.49\cdot10^{-4}$ (R; Ref. 100)	$9.1\cdot10^{-4}$
374.2	287 (Ref. 3)	$1.02\cdot10^{-3}$ (T; Ref. 3)	$9.2\cdot10^{-4}$
398.0	577 (Ref. 3)	$1.40\cdot10^{-3}$ (T; Ref. 3)	$1.4\cdot10^{-3}$
420.9	1053 (Ref. 3)	$2.17\cdot10^{-3}$ (T; Ref. 3)	$2.1\cdot10^{-3}$
423.0	1073 (Ref. 3), 6500 (Ref. 68)	$2.28\cdot10^{-3}$ (R; Ref. 3), $2.20\cdot10^{-3}$ (R; Ref. 68)	$2.2\cdot10^{-3}$
423.2	1054.9 (Ref. 100)	$2.42\cdot10^{-3}$ (T; Ref. 100)	$2.2\cdot10^{-3}$
426.2		$2.978\cdot10^{-3}$ (D; Ref. 40)	$2.3\cdot10^{-3}$
448.0	1901 (Ref. 3)	$3.49\cdot10^{-3}$ (T; Ref. 3)	$3.4\cdot10^{-3}$
448.6	1859 (Ref. 3)	$3.40\cdot10^{-3}$ (T; Ref. 3)	$3.5\cdot10^{-3}$
451.2		$5.044\cdot10^{-3}$ (D; Ref. 40)	$3.6\cdot10^{-3}$
473.0	6500 (Ref. 68)	$5.00\cdot10^{-3}$ (T; Ref. 68)	$5.5\cdot10^{-3}$
473.2	2700 (Ref. 23) 3020 (Ref. 100)	$5.74\cdot10^{-3}$ (T; Ref. 23), $5.40\cdot10^{-3}$ (T; Ref. 100)	$5.5\cdot10^{-3}$
473.4	3045 (Ref. 3)	$5.64\cdot10^{-3}$ (T; Ref. 3)	$5.6\cdot10^{-3}$
477.0	3218 (Ref. 3)	$6.07\cdot10^{-3}$ (T; Ref. 3)	$6.0\cdot10^{-3}$
477.2		$6.844\cdot10^{-3}$ (T; Ref. 40)	$6.0\cdot10^{-3}$
498.2	4100 (Ref. 23)	$9.12\cdot10^{-3}$ (R; Ref. 23), $9.00\cdot10^{-3}$ (R; Ref. 40)	$8.9\cdot10^{-3}$
514.2		$1.067\cdot10^{-2}$ (T; Ref. 40)	$1.2\cdot10^{-2}$
523.2	6600 (Ref. 23)	$1.54\cdot10^{-2}$ (T; Ref. 23)	$1.4\cdot10^{-2}$
527.2		$1.217\cdot10^{-2}$ (T; Ref. 40)	$1.5\cdot10^{-2}$

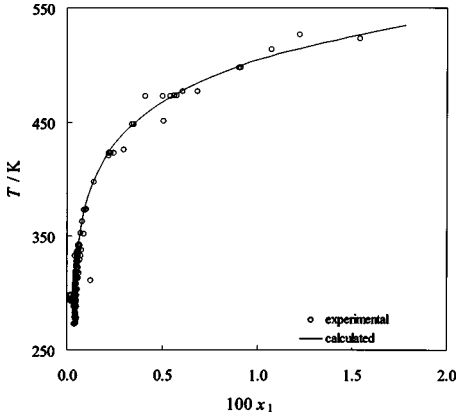

FIG. 3. All the solubility data for benzene (1) in water (2).

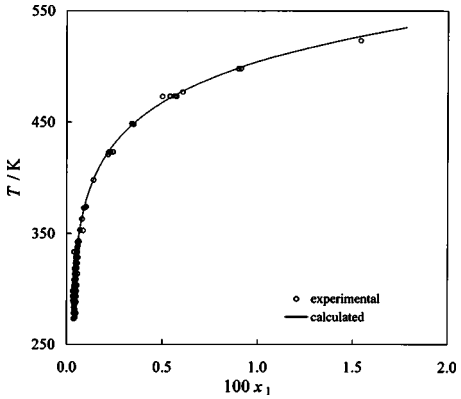

FIG. 4. Recommended and tentative solubility data for benzene (1) in water (2)

Critical Evaluation of the Solubility of Water (2) in Benzene (1)

Experimental solubility data for (2) in (1) have been reported in the 41 publications listed below together with temperature range and pressure range if reported:

Author (s)	T/K	Author (s)	T/K
Anderson and Prausnitz[3]	374–477 (287–3218 kPa)	Karlsson[50]	288–308
Barbaudy[7]	342	Kirchnerova and Cave[52]	298
Berkengeim[11]	283–323	Masterton and Gendrano[61]	298
Bittrich *et al.*[12]	293–333	McCants *et al.*[66]	311
Black *et al.*[13]	283–299	Moule and Thurston[71]	283–323
Budantseva *et al.*[20]	293	Niini[72]	293
Burd and Braun[21]	359–473 (170–2760 kPa)	Pavia[74]	282–338
Caddock and Davies[22]	293	Polak and Lu[76]	273–298
Chen and Wagner[24]	303–373 (100–350 kPa)	Robertson[79]	279
Clifford[26]	294–328	Roddy and Coleman[80]	298
Donahue and Bartell[29]	298	Rosenbaum and Walton[81]	283–333
Englin *et al.*[31]	273–323	Schatzberg[89]	293
Goldman[34]	283–313	Singh and Sah[91]	303
Gramajo de Doz *et al.*[35]	303	Staveley *et al.*[93]	298–344
Gregory *et al.*[36]	308	Staveley *et al.*[94]	296–346
Griswold *et al.*[37]	298–323	Stephenson[96]	298
Groschuff[38]	276–350	Tarassenkow and Poloshinzewa[98]	278–346
Hill[44]	279–343	Thompson and Snyder[99]	311–476 (7000 kPa)
Högfeldt and Bolander[45]	298	Tsonopoulos and Wilson[100]	313–473 (31–3020 kPa)
Johnson *et al.*[48]	298	Uspenskii[102]	283–295
Jones and Monk[49]	298–308	Wing and Johnston[104]	298

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface and expressed by Eq. (2)

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \tag{2}$$

where $d_1 = -0.509$; $d_2 = -4.316$; $d_3 = -0.203$; $d_4 = -3.637$; $T_r = T/541.7$.

In contrast to the smoothed equation used by Hefter and Young[125] for regression of the solubility data of water in benzene, Eq. (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of benzene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 3.

The experimental and reference solubility data for (2) in (1) are listed in Table 4 and shown in Fig. 5. The recommended and tentative data are shown in Fig. 6.

TABLE 3. The data categories for solubility of water (2) in benzene (1)

T/K	Recommended (data in good agreement with each other and with the reference data)	Tentative (data in good agreement with the reference data)	Doubtful (data in poor agreement with the reference data)
273.2		Polak and Lu[76]	Englin *et al.*[31]
276.2		Groschuff[38]	
278.2			Tarassenkow and Poloshinzewa[98]
278.6	Hill[44] Robertson[79]		
282.4		Pavia[74]	
282.6		Moule and Thurston[71]	
282.7		Tarassenkow and Poloshinzewa[98]	
283.2	Berkengeim[11] Englin *et al.*[31] Goldman[34] Rosenbaum and Walton[81]	Black *et al.*[13] Uspenskii[102]	
287.7		Tarassenkow and Poloshinzewa[98]	
288.1	Karlsson,[50] Moule and Thurston[71]		
288.2	Goldman[34] Hill[44]		
291.1		Karlsson[50]	
293.2	Bittrich *et al.*[12] Budantseva *et al.*[20] Englin *et al.*[31] Goldman[34] Niini[72] Pavia[7] Rosenbaum and Walton[81]	Berkengeim[11] Black *et al.*[13] Caddock and Davies[22] Karlsson[50] Schatzberg[89]	
293.3		Moule and Thurston[71]	
294.2		Clifford[26]	

295.2		Uspenskii[102]	
295.7		Tarassenkow and Poloshinzewa[98]	
295.9		Staveley *et al.*[94]	
296.1		Karlsson[50]	
296.2		Groschuff[38]	
297.7		Moule and Thurston[71]	
297.9		Staveley *et al.*[93]	
298.1		Karlsson[50]	
298.2	Donahue and Bartell[29] Goldman[34] Högfeldt and Bolander[45] Johnson *et al.*[48] Kirchnerova and Cave[52] Masterton and Gendrano[61] Polak and Lu[76] Stephenson[96]	Griswold *et al.*[37] Hill[44] Jones and Monk[49] Roddy and Coleman[80] Stephenson[96]	Wing and Johnston[104]
299.2		Black *et al.*[13]	
299.8		Clifford[26]	
301.1		Karlsson[50]	
302.7		Moule and Thurston[71]	
303.1		Karlsson[50]	
303.2	Goldman[34] Singh and Sah[91]	Berkengeim[11] Chen and Wagner[24] Englin *et al.*[31] Jones and Monk[49] Rosenbaum and Walton[81]	Gramajo de Doz *et al.*[35]
303.3		Pavia[74]	
303.7		Staveley *et al.*[94]	
305.1		Karlsson[50]	
305.2		Tarassenkow and Poloshinzewa[98]	
306.2		Staveley *et al.*[94]	
308.0		Moule and Thurston[71]	
308.2	Goldman[34] Gregory *et al.*[36]	Jones and Monk[49] Karlsson[50]	
310.7		Hill[44]	
310.9		Thompson and Snyder[99]	
311.0		Thompson and Snyder[99]	McCants *et al.*[66]
311.1		Thompson and Snyder[99]	
311.5		Thompson and Snyder[99]	
311.8		Thompson and Snyder[99]	
313.2	Wagner[24] Goldman[34] Groschuff[38] Tsonopoulos and Wilson[100]	Berkengeim[11] Chen and Englin *et al.*[31] Moule and Thurston[71] Rosenbaum and Walton[81] Tarassenkow and Poloshinzewa[98]	Bittrich *et al.*[12]
313.3		Pavia[74]	
313.8		Staveley *et al.*[94]	
314.6		Staveley *et al.*[93]	
315.1		Staveley *et al.*[94]	
315.2		Clifford[26]	
316.9		Moule and Thurston[71]	
317.2		Staveley *et al.*[93]	
319.1		Staveley *et al.*[94]	
322.6		Moule and Thurston[71]	
323.1		Pavia[74]	
323.2	Griswold *et al.*[37] Hill[44]	Berkengeim[11] Chen and Wagner[24] Englin *et al.*[31] Rosenbaum and Walton[81]	
323.6		Staveley *et al.*[93]	
325.1		Staveley *et al.*[94]	
325.4		Staveley *et al.*[94]	
326.4		Staveley *et al.*[94]	
327.9		Staveley *et al.*[94]	
328.2		Groschuff[38]	Clifford[26]
329.2		Tarassenkow and Poloshinzewa[98]	
330.7		Hill[44]	
331.4		Staveley *et al.*[93]	
331.7		Staveley *et al.*[93]	
333.1		Pavia[74]	
333.2		Chen and Wagner[24] Rosenbaum and Walton[81]	Bittrich *et al.*[12]
334.1		Staveley *et al.*[94]	
338.2	Hill[44] Pavia[74]		
338.5		Staveley *et al.*[94]	
339.2		Groschuff[38]	
340.4		Staveley *et al.*[94]	
340.7		Tarassenkow and Poloshinzewa[98]	
342.4			Barbaudy[7]
342.7		Hill[44]	
343.2		Chen and Wagner[24]	
344.2		Staveley *et al.*[93]	
344.4		Thompson and Snyder[99]	
346.2		Tarassenkow and Poloshinzewa[98]	
346.4		Staveley *et al.*[94]	
350.2		Groschuff[38]	
353.2		Chen and Wagner[24]	
359.0		Burd and Braun[21]	
363.2		Chen and Wagner[24]	
373.2		Chen and Wagner[24] Tsonopoulos and Wilson[100]	
374.2		Anderson and Prausnitz[3]	
377.0		Thompson and Snyder[99]	
385.0		Burd and Braun[21]	
398.0		Anderson and Prausnitz[3]	
411.0		Thompson and Snyder[99]	
413.0		Burd and Braun[21]	
420.9		Anderson and Prausnitz[3]	
423.0		Anderson and Prausnitz[3]	
423.2		Tsonopoulos and Wilson[100]	
434.0		Burd and Braun[21]	
443.0			Burd and Braun[21]
444.3		Thompson and Snyder[99]	
448.0		Anderson and Prausnitz[3]	
448.6		Anderson and Prausnitz[3]	
453.0			Burd and Braun[21]
461.0			Burd and Braun[21]
469.0			Burd and Braun[21]
473.0			Burd and Braun[21]
473.2	Chandler *et al.*[23] Tsonopoulos and Wilson[100]		
473.4		Anderson and Prausnitz[3]	
476.1		Thompson and Snyder[99]	
477.0		Anderson and Prausnitz[3]	
498.2		Chandler *et al.*[23]	
523.2		Chandler *et al.*[23]	

TABLE 4. Experimental values for solubility of water (2) in benzene (1)

T/K	P/kPa	Experimental values x_2 (R=recommended, T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2		$1.73\cdot10^{-3}$ (D; Ref. 31), $1.31\cdot10^{-3}$ (T; Ref. 76)	$1.2\cdot10^{-3}$
276.2		$1.30\cdot10^{-3}$ (T; Ref. 38)	$1.4\cdot10^{-3}$
278.2		$1.00\cdot10^{-3}$ (D; Ref. 98)	$1.5\cdot10^{-3}$
278.6		$1.50\cdot10^{-3}$ (R; Ref. 44), $1.50\cdot10^{-3}$ (R; Ref. 79)	$1.5\cdot10^{-3}$
282.4		$1.783\cdot10^{-3}$ (T; Ref. 74)	$1.7\cdot10^{-3}$
282.6		$1.92\cdot10^{-3}$ (T; Ref. 71)	$1.7\cdot10^{-3}$
282.7		$1.50\cdot10^{-3}$ (T; Ref. 98)	$1.7\cdot10^{-3}$
283.2		$1.70\cdot10^{-3}$ (R; Ref. 11), $1.30\cdot10^{-3}$ (T; Ref. 13), $1.93\cdot10^{-3}$ (R; Ref. 31), $1.91\cdot10^{-3}$ (R; Ref. 34), $1.95\cdot10^{-3}$ (R; Ref. 81), $2.20\cdot10^{-3}$ (T; Ref. 102)	$1.8\cdot10^{-3}$
287.7		$1.80\cdot10^{-3}$ (T; Ref. 98)	$2.1\cdot10^{-3}$
288.1		$2.31\cdot10^{-3}$ (R; Ref. 50), $2.30\cdot10^{-3}$ (R; Ref. 71)	$2.1\cdot10^{-3}$
288.2		$2.26\cdot10^{-3}$ (R; Ref. 34), $2.30\cdot10^{-3}$ (R; Ref. 44)	$2.1\cdot10^{-3}$
291.1		$2.56\cdot10^{-3}$ (T; Ref. 50)	$2.3\cdot10^{-3}$
293.2		$2.30\cdot10^{-3}$ (T; Ref. 11), $2.54\cdot10^{-3}$ (R; Ref. 12), $1.84\cdot10^{-3}$ (T; Ref. 13), $1.93\cdot10^{-3}$ (T; Ref. 13), $2.40\cdot10^{-3}$ (R; Ref. 20), $2.20\cdot10^{-3}$ (T; Ref. 22), $2.52\cdot10^{-3}$ (R; Ref. 31), $2.67\cdot10^{-3}$ (R; Ref. 34), $2.74\cdot10^{-3}$ (T; Ref. 50), $2.60\cdot10^{-3}$ (R; Ref. 72), $2.592\cdot10^{-3}$ (R; Ref. 74), $2.629\cdot10^{-3}$ (R; Ref. 74), $2.48\cdot10^{-3}$ (R; Ref. 81), $2.30\cdot10^{-3}$ (T; Ref. 89)	$2.5\cdot10^{-3}$
293.3		$2.77\cdot10^{-3}$ (T; Ref. 71)	$2.5\cdot10^{-3}$
294.2		$2.00\cdot10^{-3}$ (T; Ref. 26)	$2.6\cdot10^{-3}$
295.2		$2.90\cdot10^{-3}$ (T; Ref. 102)	$2.7\cdot10^{-3}$
295.7		$2.60\cdot10^{-3}$ (T; Ref. 98)	$2.7\cdot10^{-3}$
295.9		$2.606\cdot10^{-3}$ (T; Ref. 94)	$2.7\cdot10^{-3}$
296.1		$2.98\cdot10^{-3}$ (T; Ref. 50)	$2.8\cdot10^{-3}$
296.2		$2.60\cdot10^{-3}$ (T; Ref. 38)	$2.8\cdot10^{-3}$
297.7		$3.14\cdot10^{-3}$ (T; Ref. 71)	$2.9\cdot10^{-3}$
297.9		$2.96\cdot10^{-3}$ (T; Ref. 93)	$2.9\cdot10^{-3}$
298.1		$3.14\cdot10^{-3}$ (T; Ref. 50)	$2.9\cdot10^{-3}$
298.2		$3.10\cdot10^{-3}$ (R; Ref. 29), $3.14\cdot10^{-3}$ (R; Ref. 34), $2.60\cdot10^{-3}$ (T; Ref. 37), $3.20\cdot10^{-3}$ (T; Ref. 44), $2.90\cdot10^{-3}$ (R; Ref. 45), $3.11\cdot10^{-3}$ (R; Ref. 48), $2.80\cdot10^{-3}$ (T; Ref. 49), $3.11\cdot10^{-3}$ (R; Ref. 52), $3.09\cdot10^{-3}$ (R; Ref. 61), $2.99\cdot10^{-3}$ (R; Ref. 76), $3.23\cdot10^{-3}$ (T; Ref. 80), $2.90\cdot10^{-3}$ (R; Ref. 96), $3.29\cdot10^{-3}$ (T; Ref. 96), $4.90\cdot10^{-3}$ (D; Ref. 104)	$3.0\cdot10^{-3}$
299.2		$2.34\cdot10^{-3}$ (T; Ref. 13)	$3.1\cdot10^{-3}$
299.8		$2.40\cdot10^{-3}$ (T; Ref. 26)	$3.1\cdot10^{-3}$
301.1		$3.47\cdot10^{-3}$ (T; Ref. 50)	$3.3\cdot10^{-3}$
302.7		$3.67\cdot10^{-3}$ (T; Ref. 71)	$3.4\cdot10^{-3}$
303.1		$3.70\cdot10^{-3}$ (T; Ref. 50)	$3.5\cdot10^{-3}$
303.2	100 (Ref. 24)	$2.90\cdot10^{-3}$ (T; Ref. 11), $3.84\cdot10^{-3}$ (T; Ref. 24), $3.24\cdot10^{-3}$ (T; Ref. 31), $3.55\cdot10^{-3}$ (R; Ref. 34), $1.70\cdot10^{-3}$ (D; Ref. 35), $3.20\cdot10^{-3}$ (T; Ref. 49), $3.22\cdot10^{-3}$ (T; Ref. 81), $3.50\cdot10^{-3}$ (R; Ref. 91)	$3.5\cdot10^{-3}$
303.3		$3.597\cdot10^{-3}$ (T; Ref. 74)	$3.5\cdot10^{-3}$
303.7		$3.674\cdot10^{-3}$ (T; Ref. 94)	$3.5\cdot10^{-3}$
305.1		$3.97\cdot10^{-3}$ (T; Ref. 50)	$3.7\cdot10^{-3}$
305.2		$3.50\cdot10^{-3}$ (T; Ref. 98)	$3.7\cdot10^{-3}$
306.2		$3.784\cdot10^{-3}$ (T; Ref. 94)	$3.8\cdot10^{-3}$
308.0		$4.40\cdot10^{-3}$ (T; Ref. 71)	$4.1\cdot10^{-3}$
308.2		$4.23\cdot10^{-3}$ (R; Ref. 34), $4.19\cdot10^{-3}$ (R; Ref. 36), $3.70\cdot10^{-3}$ (T; Ref. 49), $4.43\cdot10^{-3}$ (T; Ref. 50)	$4.1\cdot10^{-3}$
310.7		$5.00\cdot10^{-3}$ (T; Ref. 44)	
310.9	7000 (Ref. 99)	$4.18\cdot10^{-3}$ (T; Ref. 99), $4.16\cdot10^{-3}$ (T; Ref. 99)	$4.4\cdot10^{-3}$
311.0	7000 (Ref. 99)	$1.30\cdot10^{-3}$ (D; Ref. 66), $4.66\cdot10^{-3}$ (T; Ref. 99)	$4.5\cdot10^{-3}$
311.1	7000 (Ref. 99)	$4.87\cdot10^{-3}$ (T; Ref. 99)	$4.5\cdot10^{-3}$
311.5	7000 (Ref. 99)	$4.21\cdot10^{-3}$ (T; Ref. 99)	$4.5\cdot10^{-3}$
311.8	7000 (Ref. 99)	$4.33\cdot10^{-3}$ (T; Ref. 99)	$4.6\cdot10^{-3}$
313.2	100 (Ref. 24), 30.54 (Ref. 100)	$3.60\cdot10^{-3}$ (Ref. 11), $3.08\cdot10^{-3}$ (Ref. 12), $4.74\cdot10^{-3}$ (Ref. 24), $4.10\cdot10^{-3}$ (Ref. 31), $4.76\cdot10^{-3}$ (Ref. 34), $4.90\cdot10^{-3}$ (Ref. 38), $5.09\cdot10^{-3}$ (Ref. 71), $4.12\cdot10^{-3}$ (Ref. 81), $4.40\cdot10^{-3}$ (Ref. 98), $4.71\cdot10^{-3}$ (Ref. 100), $5.01\cdot10^{-3}$ (Ref. 100)	$4.8\cdot10^{-3}$
313.3		$4.845\cdot10^{-3}$ (Ref. 74)	$4.8\cdot10^{-3}$
313.8		$5.041\cdot10^{-3}$ (T; Ref. 94)	$4.9\cdot10^{-3}$
314.6		$5.23\cdot10^{-3}$ (T; Ref. 93)	$5.0\cdot10^{-3}$
315.1		$5.153\cdot10^{-3}$ (T; Ref. 94)	$5.1\cdot10^{-3}$
315.2		$3.80\cdot10^{-3}$ (T; Ref. 26)	$5.1\cdot10^{-3}$
316.9		$5.76\cdot10^{-3}$ (T; Ref. 71)	$5.3\cdot10^{-3}$
317.2		$5.88\cdot10^{-3}$ (T; Ref. 93)	$5.4\cdot10^{-3}$
319.1		$6.064\cdot10^{-3}$ (T; Ref. 94)	$5.7\cdot10^{-3}$
322.6		$6.78\cdot10^{-3}$ (T; Ref. 71)	$6.3\cdot10^{-3}$
323.1		$6.567\cdot10^{-3}$ (T; Ref. 74)	$6.4\cdot10^{-3}$
323.2	100 (Ref. 24)	$4.90\cdot10^{-3}$ (T; Ref. 11), $7.23\cdot10^{-3}$ (T; Ref. 24), $5.09\cdot10^{-3}$ (T; Ref. 31), $6.50\cdot10^{-3}$ (R; Ref. 37), $6.70\cdot10^{-3}$ (R; Ref. 44), $5.48\cdot10^{-3}$ (T; Ref. 81)	$6.4\cdot10^{-3}$
323.6		$6.97\cdot10^{-3}$ (T; Ref. 93)	$6.5\cdot10^{-3}$
325.1		$6.902\cdot10^{-3}$ (T; Ref. 94)	$6.8\cdot10^{-3}$
325.4		$7.078\cdot10^{-3}$ (T; Ref. 94)	$6.9\cdot10^{-3}$
326.4		$7.211\cdot10^{-3}$ (T; Ref. 94)	$7.1\cdot10^{-3}$
327.9		$7.521\cdot10^{-3}$ (T; Ref. 94)	$7.4\cdot10^{-3}$
328.2		$4.90\cdot10^{-3}$ (D; Ref. 26), $7.90\cdot10^{-3}$ (T; Ref. 38)	$7.4\cdot10^{-3}$
329.2		$7.80\cdot10^{-3}$ (T; Ref. 98)	$7.7\cdot10^{-3}$
330.7		$8.00\cdot10^{-3}$ (T; Ref. 44)	$8.0\cdot10^{-3}$
331.4		$8.91\cdot10^{-3}$ (T; Ref. 93)	$8.2\cdot10^{-3}$
331.7		$9.41\cdot10^{-3}$ (T; Ref. 93)	$8.2\cdot10^{-3}$
333.1		$8.657\cdot10^{-3}$ (T; Ref. 74)	$8.5\cdot10^{-3}$
333.2	150 (Ref. 24)	$3.72\cdot10^{-3}$ (D; Ref. 12), $9.50\cdot10^{-3}$ (T; Ref. 24), $7.05\cdot10^{-3}$ (T; Ref. 81)	$8.6\cdot10^{-3}$
334.1		$9.294\cdot10^{-3}$ (T; Ref. 94)	$8.8\cdot10^{-3}$
338.2		$9.90\cdot10^{-3}$ (R; Ref. 44), $9.73\cdot10^{-3}$ (R; Ref. 74)	$9.8\cdot10^{-3}$
338.5		$1.05\cdot10^{-2}$ (T; Ref. 94)	$9.9\cdot10^{-3}$
339.2		$1.10\cdot10^{-2}$ (T; Ref. 38)	$1.0\cdot10^{-2}$
340.4		$1.121\cdot10^{-2}$ (T; Ref. 94)	$1.0\cdot10^{-2}$
340.7		$1.08\cdot10^{-2}$ (T; Ref. 98)	$1.1\cdot10^{-2}$
342.4		$1.20\cdot10^{-3}$ (D; Ref. 7)	$1.1\cdot10^{-2}$
342.7		$1.14\cdot10^{-2}$ (T; Ref. 44)	$1.1\cdot10^{-2}$
343.2	250 (Ref. 24)	$1.22\cdot10^{-2}$ (T; Ref. 24)	$1.1\cdot10^{-2}$
344.2		$1.274\cdot10^{-2}$ (T; Ref. 93)	$1.2\cdot10^{-2}$
344.4	7000 (Ref. 99)	$1.24\cdot10^{-2}$ (T; Ref. 99)	$1.2\cdot10^{-2}$
346.2		$1.29\cdot10^{-2}$ (T; Ref. 98)	$1.2\cdot10^{-2}$
346.4		$1.302\cdot10^{-2}$ (T; Ref. 94)	$1.2\cdot10^{-2}$
350.2		$1.45\cdot10^{-2}$ (T; Ref. 38)	$1.4\cdot10^{-2}$
353.2	250 (Ref. 24)	$1.54\cdot10^{-2}$ (T; Ref. 24)	$1.5\cdot10^{-2}$
359.0	170 (Ref. 21)	$1.40\cdot10^{-2}$ (T; Ref. 21)	$1.7\cdot10^{-2}$
363.2	350 (Ref. 24)	$2.07\cdot10^{-2}$ (T; Ref. 24)	$1.9\cdot10^{-2}$
373.2	350 (Ref. 24), 275.8 (Ref. 100)	$2.65\cdot10^{-2}$ (T; Ref. 24), $1.81\cdot10^{-2}$ (T; Ref. 100), $2.08\cdot10^{-2}$ (T; Ref. 100)	$2.4\cdot10^{-2}$
374.2	287 (Ref. 3)	$2.135\cdot10^{-2}$ (T; Ref. 3)	$2.5\cdot10^{-2}$

377.0	7000 (Ref. 99)	$2.74\cdot10^{-2}$ (T; Ref. 99)	$2.6\cdot10^{-2}$
385.0	340 (Ref. 21)	$2.70\cdot10^{-2}$ (T; Ref. 21)	$3.2\cdot10^{-2}$
398.0	577 (Ref. 3)	$3.658\cdot10^{-2}$ (T; Ref. 3)	$4.2\cdot10^{-2}$
411.0	7000 (Ref. 99)	$5.580\cdot10^{-2}$ (T; Ref. 99)	$5.6\cdot10^{-2}$
413.0	690 (Ref. 21)	$4.50\cdot10^{-2}$ (T; Ref. 21)	$5.8\cdot10^{-2}$
420.9	1053 (Ref. 3)	$6.081\cdot10^{-2}$ (T; Ref. 3)	$6.8\cdot10^{-2}$
423.0	1073 (Ref. 3)	$6.513\cdot10^{-2}$ (T; Ref. 3)	$7.1\cdot10^{-2}$
423.2	1054.9 (Ref. 100)	$7.13\cdot10^{-2}$ (T; Ref. 100)	$7.2\cdot10^{-2}$
434.0	1030 (Ref. 21)	$6.40\cdot10^{-2}$ (T; Ref. 21)	$8.9\cdot10^{-2}$
443.0	1380 (Ref. 21)	$7.20\cdot10^{-2}$ (D; Ref. 21)	$1.1\cdot10^{-1}$
444.3	7000 (Ref. 99)	$1.00\cdot10^{-1}$ (T; Ref. 99)	$1.1\cdot10^{-1}$
448.0	1901 (Ref. 3)	$1.058\cdot10^{-1}$ (T; Ref. 3)	$1.2\cdot10^{-1}$
448.6	1859 (Ref. 3)	$1.053\cdot10^{-1}$ (T; Ref. 3)	$1.2\cdot10^{-1}$
453.0	1720 (Ref. 21)	$8.40\cdot10^{-2}$ (D; Ref. 21)	$1.3\cdot10^{-1}$
461.0	2070 (Ref. 21)	$9.10\cdot10^{-2}$ (D; Ref. 21)	$1.5\cdot10^{-1}$
469.0	2410 (Ref. 21)	$1.04\cdot10^{-1}$ (D; Ref. 21)	$1.7\cdot10^{-1}$
473.0	2760 (Ref. 21)	$1.11\cdot10^{-1}$ (D; Ref. 21)	$1.8\cdot10^{-1}$
473.2	2700 (Ref. 23), 3020 (Ref. 100)	$1.88\cdot10^{-1}$ (R; Ref. 23), $1.85\cdot10^{-1}$ (R; Ref. 100)	$1.8\cdot10^{-1}$
473.4	3045 (Ref. 3)	$1.792\cdot10^{-1}$ (T; Ref. 3)	$1.8\cdot10^{-1}$
476.1	7000 (Ref. 99)	$1.77\cdot10^{-1}$ (T; Ref. 99)	$1.9\cdot10^{-1}$
477.0	3218 (Ref. 3)	$1.886\cdot10^{-1}$ (T; Ref. 3)	$2.0\cdot10^{-1}$
498.2	4100 (Ref. 23)	$2.23\cdot10^{-1}$ (T; Ref. 23)	$2.8\cdot10^{-1}$
523.2	6600 (Ref. 23)	$3.94\cdot10^{-1}$ (T; Ref. 23)	$4.3\cdot10^{-1}$

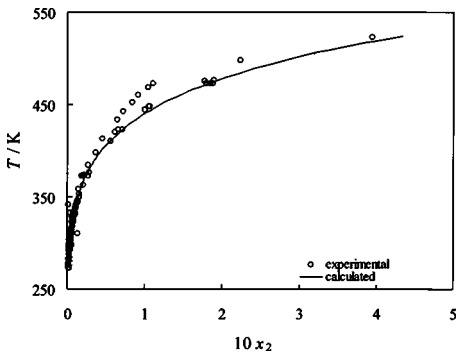

FIG. 5. All the solubility data for water (2) in benzene (1).

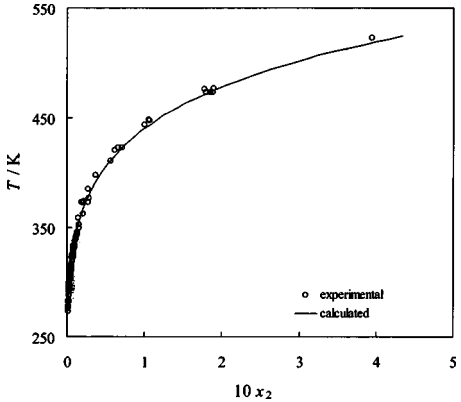

FIG. 6. Recommended and tentative solubility data for water (2) in benzene (1).

High Pressure Solubility of Benzene (1) in Water (2)

The experimental high pressure solubility for (1) in (2) investigated by the authors listed below have not been critically evaluated because the developed method is not applicable for such data. Hefter and Young[125] have presented an evaluation of these data.

Author (s)	T/K	P/kPa	Author (s)	T/K	P/kPa
Alwani and Schneider[2]	567–636		O'Grady[73]	561–566	24 900
Bradley *et al.*[17]	318–328	62 500	Kudchadker and McKetta[57]	311–411	109–5672
Chandler *et al.*[23]	523–548	17 200	Rebert and Kay[78]	561–580	12 160–15 870
Connolly[27]	533–573	10 100–81 100	Sawamura *et al.*[87]	298	100–100 000
Filyas[32]	568	1010	Skripka[92]	498–533	4700–78 500
Jäger[46]	373–573		Thompson and Snyder[99]	311–511	34 600
Miller and Hawthorne[68]	298 and 473	40 000			

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[116] are independent data. The data reported by Ben-Naim *et al.*,[8] Alwani and Schneider,[106] Durand,[107] Gill *et al.*,[108] Green and Frank,[111] Hicks and Young,[113] Joris and Taylor,[115] McAuliffe,[117] Roof,[118] and Scott and van Konynenburg,[120] lack sufficient information to justify evaluation. Therefore these data are rejected. The publications of Gorbachev *et al.*,[109,110] Herz,[112] Horiba,[114] Scheffer,[119] Sultanov and Skripka,[121] Thompson,[122] Umano and Hayano,[123] and Vermilion[124] were not accessible to the compilers.

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Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. W. Alexander, J. Phys. Chem. **63**, 1021 (1959).

Variables:
Temperature: 0.8 °C–65.4 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values
Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln
0.8	4.25	0.184[a]
9.4	4.13	0.179
16.8	4.09	0.177
24.0	4.16	0.180
31.0	4.23	0.183
38.0	4.50	0.192
44.7	4.69	0.203
51.5	4.94	0.214
58.8	5.40	0.234
65.4	5.94	0.257

[a]Supercooled liquid.

Auxiliary Information

Method/Apparatus/Procedure:
The method was based on that of Bohon and Claussen.[1] Absorbance was determined with a Beckman model D.U. ultraviolet spectrophotometer.

Source and Purity of Materials:
(1) Analar benzene; shaken with mercury and purified according to the method of Mair *et al.*[2]
(2) Not specified.

Estimated Error:
Solubility: ±0.5% (type of error was not specified).

References:
[1]R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).
[2]J. Mair, D. J. Termini, C. B. Willingham, and F. D. Rossini, J. Research Natl. Bur. Standards **37**, 229 (1946).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Z. Alwani and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **73**, 294 (1969).

Variables:
Critical temperature and critical pressure

Prepared By:
C. L. Young

Experimental Values
Values of critical temperatures and pressures

t/°C	T/K	P/bar
339.5	612.7	2000
329.7	602.9	1600
320.2	593.4	1200
309.5	582.7	800
297.1	570.3	400
294.2	567.4	200
297.4	570.6	170
304.9	578.1	154
325.4	598.6	171
363.0	636.2	210

Auxiliary Information

Method/Apparatus/Procedure:
Measurements were made in a steel optical cell in large aluminum block furnace. The cell contents were stirred by a magnetically operated stirrer. The pressure was measured using a movable piston and Bourdon gauge. The temperature was measured using a steel-sheathed thermocouple. Components were charged into the cell and one phase-two phase boundaries were observed visually. Critical properties were determined from boundary envelopes.

Source and Purity of Materials:
(1) Analytical grade product fractionally distilled, purity 99.9 mole %.
(2) Distilled and degassed.

Estimated Error:
Temperature: ΔT/K = 0.4.
Pressure: $\Delta P/P = \pm 0.02$ (estimated by compiler).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. E. Anderson and J. M. Prausnitz, Fluid Phase Equilib. **32**, 63 (1986).

Variables:
Temperature: 101.0 °C–203.8 °C
Pressure: 2.87 bar–32.18 bar

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

t/°C	P/bar	g (1)/100 g sln (compilers)	$10^3 \cdot x_1$
101.0	2.87	0.441	1.02 ± 0.035
124.8	5.77	0.604	1.40 ± 0.047
147.7	10.53	0.934	2.17 ± 0.042
149.8	10.73	0.981	2.28 ± 0.040
174.8	19.01	1.499	3.49 ± 0.014
175.4	18.59	1.458	3.40 ± 0.055
200.2	30.45	2.400	5.64 ± 0.350
203.8	32.18	2.580	6.07 ± 0.092

Solubility of water in benzene

t/°C	P/bar	g (2)/100 g sln (compilers)	x_2
101.0	2.87	0.5006	0.02135 ± 0.00045
124.8	5.77	0.8681	0.03658 ± 0.00068
147.7	10.53	1.471	0.06081 ± 0.00034
149.8	10.73	1.581	0.06513 ± 0.00074
174.8	19.01	2.656	0.1058 ± 0.00190
175.4	18.59	2.643	0.1053 ± 0.00160
200.2	30.45	4.794	0.1792 ± 0.00060
203.8	32.18	5.088	0.1886 ± 0.00073

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The equilibrium cell, about 140 mL, was filled with a mixture of (1) and (2), temperature controllers were set at the desire temperature, liquids were degassed, agitated and allowed to reach equilibrium for 2 h. Details of the apparatus and sampling procedures were described in the paper. The temperatures were measured by a resistance temperature detector. All analyses were made using a gas chromatograph equipped with a thermal-conductivity detector. Mean values of 3–7 replicated measurements were reported.

Source and Purity of Materials:
(1) Source not specified; spectral grade reagent; used as received.
(2) Purified and deionized by adsorption on activated carbon.

Estimated Error:
Temperature: ±0.5 °C.
Solubility: standard deviation as above.
Pressure: ±0.1 bar.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 0.174 g (1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compilers is $4.02 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was rotated for 20 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:
(1) Eastman Kodak Co. Best grade; washed successively with concentrated sulfuric acid, water, and dilute sodium hydroxide; dried, and distilled, boiling point 80 °C.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. S. Arnold, C. A. Plank, E. E. Erickson, and F. P. Pike, Ind. Eng. Chem. **3**, 253 (1958).

Variables:
Temperature: 0.4 °C–69 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

Solubility of benzene in water, Solid, gaseous benzene plus water and air

t/K	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln
0.4	3.88	0.168
3.0	3.92	0.170
3.9	4.06	0.176
4.5	3.97	0.172

Solubility of benzene in water, Solid, liquid, gaseous benzene plus water and air

t/K	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln
4.9	3.97	0.172

Solubility of benzene in water, Liquid, gaseous benzene plus water and air

t/K	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln
5.6	4.02	0.174
6.7	4.02	0.174
9.0	3.99	0.173
12.5	3.97	0.172
15.0	3.99	0.173
20.0	3.95	0.171
20.6	3.97	0.172
24.8	3.95	0.171
24.9	4.02	0.174
27.3	4.02	0.174
30.0	4.09	0.177
30.0	4.06	0.176
35.0	4.20	0.182
39.9	4.34	0.188
45.0	4.55	0.197
45.0	4.53	0.196
49.8	4.71	0.204
54.5	4.97	0.215
59.8	5.22	0.226
64.8	5.57	0.241
69.0	5.67	0.260

Auxiliary Information

Method/Apparatus/Procedure:
In a thermostatted 3 L borosilicate glass flask (2) was saturated with (1), the water phase stirred very slowly, then the flask left quiescent and the saturated solution sampled repeatedly and analyzed on a Beckman model DU spectrophotometer until a constant benzene concentration response was achieved on successive days. Many details are given in the paper.

Source and Purity of Materials:
(1) Barrett Division of Allied Chemical and Dye Corp., thiophene-free, 1°; water washed and distilled; for two determinations (a) thrice crystallized.
(2) Distilled; electrical conductivity confirmed its high quality.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: 0.0028 g (1)/100 g sln (standard deviation).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).

Variables:
One temperature: 25 °C

Prepared By:
G. T. Hefter

Experimental Values

The solubility of benzene in water reported to be $2.24 \cdot 10^{-2}$ mol/L sln.

Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction, x_1, solubilities, calculated by the compiler, are 0.175 *g* (1)/100 g sln and $4.05 \cdot 10^{-4}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
Experiments were performed in sealed stainless steel centrifuge tubes. An excess of ^{14}C-labeled benzene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2 °C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10 000 rpm for 60 min in a head preequilibrated to 25 ± 0.3 °C, following which aliquots of the solution were removed for analysis by liquid scintillation counting. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

Source and Purity of Materials:
(1) ^{14}C-labeled benzene: New England Nuclear, used without further purification.
(2) Distilled.

Estimated Error:
Temperature: ± 0.2 °C.
Solubility: ± 0.7 rel. (representing one standard deviation).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Barbaudy, J. Chim. Phys. **23**, 289 (1926).

Variables:
One temperature: 69.25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 69.25 °C was reported to be 0.281 *g* (1)/100 g sln. The corresponding mole fraction, x_1, calculated by compiler is $6.49 \cdot 10^{-4}$.

The solubility of water in benzene at 69.25 °C was reported to be 0.279 *g* (2)/100 g sln. The corresponding mole fraction, x_2, calculated by compiler is 0.0120.

Auxiliary Information

Method/Apparatus/Procedure:
Sealed glass tubes were heated in a paraffinic oil bath for a long time above the cloud point and then cooled to turbidity.

Source and Purity of Materials:
(1) Poulenc, cryoscopic grade; thiophene free; dried over $CaCl_2$ and distilled; purity not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Ben-Naim and J. Wilf, J. Phys. Chem. **70**, 771 (1979).

Variables:
Temperature: 10.0 °C and 20.0 °C

Prepared by:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values
Solubility of benzene in water

t/°C	$10^2 \cdot$ mol(1)/L sln	$10^2 \cdot g$ (1)/100 g sln (compilers)	$10^4 \cdot x_1$ (compilers)
10.0	2.08	1.624	3.75
20.0	2.22	1.736	4.01

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A saturated solution was diluted several times and the absorbance measured by a Perkin-Elmer Model 450 spectrophotometer in the UV region of 200–400 m.

Source and Purity of Materials:
(1) Fluka, puriss grade, purity ⩾99.5%; used as received.
(2) Triply distilled.

Estimated Error:
Temperature: ±0.2 °C
Solubility: 1% (reproducibility of measurements).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Ben-Naim and J. Wilf, J. Phys. Chem. **84**, 583 (1980).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values
Solubility of benzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$2.33 \cdot 10^{-2}$	0.001823	$4.21 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water (2) with an excess of benzene (1) was stirred for about 48 h in a thermostat and then the two phases were allowed to separate for about 24 h. Samples were analyzed spectroscopically in the UV region by a Perkin-Elmer model 450 spectrophotometer. Confirming results were obtained through contact between water and the vapor of the solute; the method was described in Ben-Naim *et al.*[1]

Source and Purity of Materials:
(1) Fluka, puriss grade, 99.99%; used as received.
(2) Triple distilled.

Estimated Error:
Temperature: ±0.2 °C
Solubility: 1% (reproducibility of measurements).

References:
[1]A. Ben-Naim, J. Wilf, and M. Yaacobi, J. Phys. Chem. **77**, 95 (1973).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. I. Berkengeim, Zavod. Lab. **10**, 592 (1941).

Variables:
Temperature: 10 °C–50 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
10	1.7	0.040
20	2.3	0.053
30	2.9	0.066
40	3.6	0.084
50	4.9	0.114

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (2) in (1) was determined by the Karl Fischer reagent method.

Source and Purity of Materials:
(1) Source not specified; CP reagent; boiling point 80.4 °C; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H.-J. Bittrich, H. Gedan, and G. Feix, Z. Phys. Chem. (Leipzig) **260**, 1009 (1979).

Variables:
Temperature: 20 °C–40 °C

Prepared By:
A. Maczynski and A. Szafranski

Experimental Values

Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln (compiler)	mg (1)/kg (2)
20	4.133	0.1790	1790
40	4.676	0.2025	2025
60	5.641	0.2442	2442

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln (compiler)	mg (2)/kg (1)
20	2.54	0.0586	586
40	3.08	0.0712	712
60	3.72	0.0860	860

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was shaken at a specified temperature and then thermostatted for 48 h. The equilibrated phases were sampled and analyzed by flame-ionization glc using 3 m steel columns of 10% SE 30-on-Chromaton N (90 °C) and 1.5 g +10% SE 30-on-Chromaton N (120 °C) for (1) and (2), respectively.

Source and Purity of Materials:
(1) Source not specified; distilled and recrystallized; glc pure.
(2) Not specified.

Estimated Error:
Solubility: ±5% (type of error not specified).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).

Variables:
Temperature: 10 °C–26 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in benzene (at total saturation pressure of 1 atm)

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g (1)	g (2)/100 g sln (compiler)
10	1.30	0.030	0.030
20	1.84	0.0425	0.0425
20	1.93	0.0445	0.0445
26	2.34	0.054	0.054

The same data are reported in Jons and Taylor.[1]

Auxiliary Information

Method/Apparatus/Procedure:
Air saturated with radioactive water vapor was bubbled through (1) until saturation was attained. Dissolved water was separated from (1) by the absorption on calcium oxide. The tritium was transferred into the counter by equilibration with ethanol vapor. The method is described in Jons and Taylor.[1]

Source and Purity of Materials:
(1) Ohio State University under an American Petroleum Institute Project; purity not specified; used as received.
(2) Not specified.

Estimated Error:
Solubility: ±1% (type of error not specified).

References:
[1]G. G. Joris and H. S. Taylor, J. Chem. Phys. **16**, 45 (1948).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).

Variables:
Temperature: 0.4 °C–42.8 °C

Prepared By:
G. T. Hefter

Experimental Values

Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln[a] (compiler)
0.4	4.01	0.174[b]
5.2	4.17	0.181
10.0	4.15	0.180
14.9	4.10	0.178
21.0	4.13	0.179
25.0	4.13[c]	0.179[c]
25.6	4.13	0.179
30.2	4.24	0.184
34.9	4.36	0.189
42.8	4.61	0.200

[a]Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g (1)/L sln which was then converted to g (1)/100 g sln by assuming a solution density of 1.00 kg/L.

[b]Data refer to the solubility of solid (1) in (2).

[c]Given in the original paper as 1.79 g (1)/L sln.

Auxiliary Information

Method/Apparatus/Procedure:
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24 hours and then allowed to settle for at least another 24 h. Next, desired quantities of the water layer were syphoned into six glass-stoppered Erlenmeyer flasks. These six flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for absorption of (1) onto the walls of the cuvette.

Source and Purity of Materials:
(1) Baker and Adamson, purified by recrystallization from ethanol, washing, filtering through silica gel then distilling. Purity was determined by refractometry (no values given).
(2) Air-free conductivity water, no other details given.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: ±0.5% relative.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

Variables:
One temperature: 25.0 °C

Prepared By:
G. T. Hefter

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 0.16 mg (1)/100 mL (2).

The solubility of (1) in 40.0% (w/w?) aqueous sodium xylene sulfonate was also reported to be 0.37 mL (1)/100 mL sulfonate sln.

Auxiliary Information

Method/Apparatus/Procedure:
A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.02 mL. An excess of solute was added and the mixture allowed to come to equilibrium in a constant temperature bath then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute measured directly in the neck of the tube from the total added.

Source and Purity of Materials:
(1) Highest grade commercial sample available; no other details given.
(2) Distilled.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. S. Booth and H. E. Everson, Ind. Eng. Chem. **41**, 2627 (1949).

Variables:
Temperature: 25 °C and 60 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of benzene in water

t/°C	mL (1)/100 mL (2).
25	0.11
60	0.19

Auxiliary Information

Method/Apparatus/Procedure:
Stoppered Babcock tubes with necks graduated from 0 to 1.6 mL in steps 0.02 mL were used. A known volume of (2) (generally 50 mL) was added to the tube in constant water bath and weighed quantities of (1) were added to this solution. Then the mixture was separated by gentle rotation. After this treatment, the volume was determined directly

Source and Purity of Materials:
(1) Source not specified; CP or highest commercial grade; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±0.1 °C at 25 °C.
Solubility: ±0.1 mL (1)/100 mL (2).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. S. Bradley, M. J. Dew, and D. C. Munro, High Temp. -High Pressures **5**, 169 (1973).

Variables:
Temperature: 25 °C–55 °C
Pressure: 1 bar and 625 bar

Prepared By:
G. T. Hefter

Experimental Values

Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln (compiler)	mol (1)/L sln	P/bar[b]
25	4.21	0.183	0.0234	1
45	4.99	0.216	0.0277	1
55	5.49	0.238	0.0305	1
45	4.82	0.209	0.0268	625
55	5.87	0.254	0.0326	625

[a]Assuming a solution density of 1.00 kg/L at all temperatures.
[b]1 bar = 0.1 MPa exactly.

Data at other pressures are presented in graphical form. Data are also presented for the solubility of (1) in aqueous solutions of $AgNO_3$ and KNO_3 at various temperatures and pressures.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) at room temperature and pressure was determined in a stoppered 1mm silica cuvette placed in a Unicam SP500 spectrophotometer and stirred magnetically. Measurements were made until a constant concentration was reached. The value was crosschecked against a 2 L sample of saturated solution which had been equilibrated for some months.

Solubilities at higher temperatures and pressures were similarly determined in a special cell fitted into the spectrophotometer. Many details of the apparatus are given in the paper.

Source and Purity of Materials:
(1) A. R. grade, thiophene-free, no further details given.
(2) Distilled, air-free.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. P. Brady and H. Huff, J. Phys. Chem. **62**, 644 (1958).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubillity of benzene in water at 25 °C was reported to be 1.76 g (1)/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.176 g (1)/100 g sln and 4.06×10^{-4}. The compiler's calculation assumes a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) has been extrapolated from vapor pressure measurements. The vapor pressure apparatus used the same principle as that of McBain and O'Connor.[1]

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Solubility: 0.03 (standard deviation).

References:
[1]J. W. McBain and J. J. O'Connor, J. Am. Chem. Soc. **58**, 2610 (1936).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A **78**, 453 (1974).

Variables:
Temperature: 4.5 °C–20.1 °C

Prepared By:
G. T. Hefter

Experimental Values

Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln
4.5	4.25	0.184±0.0033
6.3	4.27	0.185±0.0033
7.1	4.18	0.181±0.0055
9.0	4.18	0.181±0.0034
11.8	4.09	0.177±0.0041
12.1	4.09	0.177±0.0035
15.1	4.14	0.179±0.0038
17.9	4.14	0.179±0.0038
20.1	4.07	0.176±0.0032

Errors are given as standard deviations.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 43 mL of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

Source and Purity of Materials:
(1) 99.99 mole %; source and methods or purification not specified.
(2) Distilled.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: see table above.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976); Deposited doc. VINITI 438-76 (1976).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 20 °C was reported to be $x_1 = 4 \times 10^{-4}$.
The corresponding mass percent calculated by the compiler is 0.17 g (1)/100 g sln.
The solubility of water in benzene at 20 °C was reported to be $x_2 = 0.0026$.
The corresponding mass percent calculated by the compiler is 0.060 g (2)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer method.

Source and Purity of Materials:
(1) Source not specified; pure or analytical; pure or analytical reagent grade; purity <99.9%.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. D. Burd, Jr. and W. G. Braun, Proc. Am. Pet. Inst., Div. Refin. **48**, 464 (1968).

Variables:
Temperature: 359 K–473 K
Pressure: 0.17 MPa–2.76 MPa

Prepared By:
A. Maczynski

Experimental Values

Solubility of water in benzene

t/°F	T/K (compiler)	x_2 (compiler)	g (2)/100 g sln	P/psia	P/MPa (compiler)
187	359	0.014	0.33	25	0.17
233	385	0.027	0.63	50	0.34
283	413	0.045	1.08	100	0.69
321	434	0.064	1.54	150	1.03
337	443	0.072	1.75	200	1.38
356	453	0.084	2.08	250	1.72
371	461	0.091	2.25	300	2.07
385	469	0.104	2.60	350	2.41
392	473	0.111	2.80	400	2.76

Auxiliary Information

Method/Apparatus/Procedure:
The measurements were carried out in the autoclave for vapor-liquid equilibrium determination. The solubility points were obtained by incremental addition of (2) followed by stirring, settling, sampling, and analysis. This procedure was continued until addition of water resulted in no pressure increase, indicating three-phase conditions. The samples were analyzed by glc.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; 99.0% by glc; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±0.5 °F.
Solubility: ±0.004 g (2)/100 g sln.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. D. Caddock and P. L. Davies, J. Inst. Pet. **46**, 391 (1960).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of water in benzene at 20 °C was reported to be 52 mg (2)/100 g (1).

The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.052 g (2)/100 g sln and 0.0022, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
A sample of (1) was equilibrated at 20 °C with an air stream containing a known amount of water vapor tagged with HTO. At equilibrium a sample of (1) was taken and its (2) content determined by liquid scintillation counting.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Temperature: ±0.01 °C.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
K. Chandler, B. Eason, C. L. Liotta, and C. A. Eckert, Ind. Eng. Chem. Res. **37**, 3515 (1998).

Variables:
Temperature: 200 °C–275 °C
Pressure: 27 bar–172 bar

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

t/°C	P/bar	g (1)/100 g sln (compilers)	$10^2 \cdot x_1$
200	27	2.44	0.574±0.019
225	41	3.84	0.912±0.078
250	66	6.35	1.54±0.09
250	172[a]	7.86	1.93±0.10
275	95	10.48	2.63±0.16
275	172[a]	9.97	2.49±0.09

Solubility of water in benzene

t/°C	P/bar	g (2)/100 g sln (compilers)	x_2
200	27	5.07	0.188±0.017
225	41	6.21	0.223±0.009
250	66	13.04	0.394±0.018
250	172[a]	15.29	0.439±0.012
275	95	23.56	0.572±0.020
275	172[a]	20.90	0.534±0.015

[a]Pressure above the three phase pressure.

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A commercially available 300 mL stainless steel sample cylinder (Whitey Co.) as an equilibrium cell, a temperature controller (Omega Engineering, Inc.) and a digital pressure transducer (Heise, 901B) were used. Details of the apparatus and sampling procedures were described in the paper. Samples were analyzed with a GLC (Varian Model 3400) equipped with a thermal conductivity detector for the water-rich phase and equipped with FID detector for the hydrocarbon-rich phase. 7–10 replicated measurements at each point were made.

Source and Purity of Materials:
Aldrich Chemicals Co.; HPLC grade reagent; purity >99.9%; used as received.
(2) Aldrich Chemicals Co.; HPLC grade water.

Estimated Error:
Temperature: ±1 °C.
Pressure: ±0.3 bar.
Solubility: standard deviation as above.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 470 (1994).

Variables:
Temperature: 303.15 K–373.15 K
Pressure: 1.0 bar–3.5 bar

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

T/K	P/bar	g (1)/100 g sln (compilers)	$10^4 \cdot x_1$
303.15	1.0	0.184	4.24±0.23
313.15	1.0	0.201	4.64±0.23
323.15	1.0	0.221	5.10±0.23
333.15	1.5	0.245	5.65±0.37
343.15	2.5	0.270	6.25±0.35
353.15	2.5	0.302	6.99±0.37
363.15	3.5	0.346	8.00±0.19
373.15	3.5	0.411	9.50±0.25

Solubility of water in benzene

T/K	P/bar	g (2)/100 g sln (compilers)	$10^2 \cdot x_2$
303.15	1.0	0.0888	0.384±0.017
313.15	1.0	0.1097	0.474±0.022
323.15	1.0	0.1677	0.723±0.056
333.15	1.5	0.2207	0.950±0.026
343.15	2.5	0.2840	1.22±0.026
353.15	2.5	0.3594	1.54±0.039
363.15	3.5	0.4851	2.07±0.039
373.15	3.5	0.6239	2.65±0.030

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The continuous flow equilibrium apparatus for mutual solubility measurements was used. The samples were collected in 25 and 60 mL vials containing 0.5–4.0 mL of dehydrated ethanol solvent. Details of the standard preparation, calibration, and sampling procedures were described in the paper. A Hewlett-Packard 5880A gas chromatograph equipped with Poropac column and a thermal conductivity detector was used for analysis. The reported solubility is the average of 6–14 replicate determinations.

Source and Purity of Materials:
(1) Aldrich Chemical Co.; spectral grade, purity >99 mole%; used as received.
(2) Distilled and deionized water.

Estimated Error:
Temperature: ±0.2 K.
Solubility: standard deviation as above.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. Chey and G. V. Calder, J. Chem. Eng. Data **17**, 199 (1972).

Variables:
One temperature: 21 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values
Solubility of benzene in water

t/°C	g (1)/100 g sln	x_1 (compilers)
21	0.174± 0.011	$4.01 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A mixture containing about 50 mL of (2) and about 1 mL of (1) was allowed to stand for 10–20 h with occasional stirring in a thermostatted separatory funnel. Procedures for sampling were described in the paper. A sample was dissolved in the isopropyl ether and was analyzed with a Carle gas chromatograph Model 8004. The mean of four experiments was reported.

Source and Purity of Materials:
(1) Source not specified; A.R. reagent; used as received.
(2) Distilled water.

Estimated Error:
Temperature: ±1 °C.
Solubility: as above.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. W. Clifford, Ind. Eng. Chem. **13**, 631 (1921).

Variables:
Temperature: 21 °C–55 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values
Solubility of benzene in water

t/°C	x_2 (compiler)	g (2)/100 g sln
21.0	0.0020	0.046
26.6	0.0024	0.055
42.0	0.0038	0.088
55.0	0.0049	0.113

Auxiliary Information

Method/Apparatus/Procedure:
A current of air predried by calcium chloride was passed through a sample. The moisture abstracted from the sample by this air was absorbed in calcium chloride tubes. The amount of water was calculated from the weights of these tubes. This method is described in Clifford.[1]

Source and Purity of Materials:
(1) Source not specified; 100% benzene; dehydrated with metallic sodium; purity not specified.
(2) Not specified.

Estimated Error:
Not specified.

References:
[1]C. W. Clifford, Ind. Eng. Chem. **13**, 628 (1921).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. F. Connolly, J. Chem. Eng. Data **11**, 13 (1966).

Variables:
Temperature: 260 °C–300 °C
Pressure: 100 atm–800 atm

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of benzene in water

t/°C	x_1 (compiler)	g (1)/100 g sln	P/atm	P/MPa (compiler)
260	0.0173	7.1	100	10.1
260	0.0178	7.3	250	25.3
260	0.0176	7.2	500	50.7
260	0.0160	6.6	800	81.1
281	0.0353	13.7	150	15.2
281	0.0356	13.8	250	25.3
281	0.0342	13.3	500	50.7
281	0.0325	12.7	600	60.8
287.5	0.0457	17.2	165	16.7
287.5	0.0485	18.1	195	19.8
287.5	0.0485	18.1	320	32.4
287.5	0.0460	17.3	380	38.5
287.5	0.0359	13.9	735	74.5
295	0.0488	18.2	135	13.7
295	0.0638	22.8	160	16.2
295	0.0786	27.0	185	18.7
295	0.0951	31.3	210	21.3
295	0.1062	34.0	225	22.8
295	0.1117	35.3	230	23.3
295	0.1126	35.5	240	24.3
295	0.1117	35.3	250	25.3
295	0.1062	34.0	265	26.8
295	0.0951	31.3	290	29.4
295	0.0786	27.0	350	35.5
295	0.0641	22.9	450	45.6
295	0.0488	18.2	690	69.9
300	0.0638	22.8	145	14.7
300	0.0797	27.3	155	15.7
300	0.0935	30.9	160	16.2
300	0.1074	34.3	160	16.2
300	0.1216	37.5	165	16.7
300	0.1332	40.0	165	16.7
300	0.1482	43.0	160	16.2
300	0.1647	46.1	160	16.2
300	0.2269	56.0	490	49.6
300	0.2031	52.5	480	48.6
300	0.1843	49.5	470	47.6
300	0.1647	46.1	470	47.6
300	0.1482	43.0	470	47.6
300	0.1332	40.0	470	47.6
300	0.1216	37.5	480	48.6
300	0.1074	34.3	490	49.6
300	0.0939	31.0	505	51.2
300	0.0797	27.3	555	56.2
300	0.0641	22.9	665	67.4

Auxiliary Information

Method/Apparatus/Procedure:
Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected until either a cloud or a small droplet of a second phase appeared at the top of the cell. Then mercury was injected to change pressure, more (1) was injected and the measurement was repeated.

Source and Purity of Materials:
(1) Phillips reagent grade better than 99.8%; used as received.
(2) Distilled and deaerated.

Estimated Error:
Temperature: ±0.02 °C.
Pressure: ±2 atm.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. C. Corby and P. H. Elworthy, J. Pharm. Pharmacol., Suppl. **23**, 39 (1971).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of benzene in water at 20 °C was reported to be 0.0218 mol·/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.170 *g* (1)/100 g sln and $3.9 \cdot 10^{-4}$. The compiler's calculation assumes a solution density of 1.00 g·/mL.

Auxiliary Information

Method/Apparatus/Procedure:
A small excess of (1) was equilibrated with (2) by shaking at 20 °C until saturation was attained. The saturated aqueous phase was analyzed by ultraviolet spectrophotometry.

Source and Purity of Materials:
(1) W. Jarvie Ltd., crystallizable; distilled before use; n_D^{18} 1.5028.
(2) Distilled once from glass.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. J. Donahue and F. E. Bartell, J. Phys. Chem. **56**, 480 (1952).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 25 °C was reported to be $x_1 = 4.2 \cdot 10^{-4}$.

The corresponding mass percent calculated by compiler is 0.182 *g* (1)/100 g sln.

The solubility of water in benzene at 25 °C was reported to be $x_2 = 0.0031$.

The corresponding mass percent calculated by compiler is 0.072 *g* (2)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:
Samples of (1) with (2) were placed in glass stoppered flasks and were shaken intermittently for at least 3 days in a water-bath held at 25 °C. The (1)-rich phases were analyzed for (2) content by the Karl-Fischer method and the (2)-rich phases were analyzed interferometrically.

Source and Purity of Materials:
(1) Source not specified; best reagent grade; purified by fractional distillation and treatment with silica gel; purity not specified.
(2) Purified.

Estimated Error:
Temperature: ±0.1 °C.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. Durand, C. R. Hebd. Seances Acad. Sci. 226, 409 (1948).

Variables:
One temperature: 16 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of benzene in water at 16 °C was reported to be 1.65 mL (1)/L (2).

Auxiliary Information

Method/Apparatus/Procedure:
The titration method described in Durand[1] was used. Addition of pipetted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.

Source and Purity of Materials:
(1) Not specified.
(2) Distilled.

Estimated Error:
Solubility: ±0.05 mL(1)/L(2)

References:
[1]R. Durand, C. R. Hebd. Seances Acad. Sci. **223**, 898 (1946).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 0 °C–50 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
0	1.730	0.03996
10	1.93	0.0446
20	2.52	0.0582
30	3.24	0.0749
40	4.10	0.0948
50	5.09	0.1177

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Yu. I. Filyas, Tr., Vses. Neftegazov. Nauch.-Issled. Inst. **45**, 68 (1973).

Variables:
One temperature: 295 °C
Pressure: 10 atm

Prepared By:
A. Maczynski

Experimental Values

The solubility of water in benzene at 295 °C and 10 atm was reported to be 0.318 g (2)/g(1).

The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 24.1 g (2)/100 g sln and 0.580 at 1.01 MPa.

Auxiliary Information

Method/Apparatus/Procedure:
Nothing is specified in the paper.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. Franks, M. Gent, and H. H. Johnson, J. Chem. Soc. 2716 (1963).

Variables:
Temperature: 17 °C–63 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of benzene in water

T/K	$10^4 \cdot x_1$	g (1)/100 g sln (compiler)
290.2	3.95	0.171
295.2	3.97	0.172
299.2	3.99	0.173
302.2	4.02	0.174
305.2	4.12	0.178
308.2	4.20	0.182
313.7	4.39	0.190
315.2	4.40	0.191
317.2	4.45	0.193
319.2	4.57	0.198
324.2	4.78	0.207
329.2	5.03	0.218
334.2	5.31	0.230
336.2	5.42	0.235

Auxiliary Information

Method/Apparatus/Procedure:
The absorbance of saturated solutions of (2) in (1) was measured directly at 254 nm on a Unicam S.P. 500 spectrophotometer.

Source and Purity of Materials:
(1) Source not specified; thiophene free; recrystallized twice from ethanol, washed, filtered through silica gel and distilled.
(2) Deionized and doubly distilled from alkaline potassium permanganate and aqueous phosphoric acid.

Estimated Error:
Temperature: ±0.05 °C.
Absorbance: ±0.5%.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Goldman, Can. J. Chem. **52**, 1668 (1974).

Variables:
Temperature: 10 °C–40 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values
Solubility of benzene in water

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln (compiler)	mol (2)/L sln
10	1.91	0.0440	0.02171
15	2.26	0.0522	0.02561
20	2.67	0.0618	0.03017
25	3.14	0.0725	0.03518
30	3.55	0.0820	0.03950
35	4.23	0.0979	0.04690
40	4.76	0.1101	0.05243

Auxiliary Information

Method/Apparatus/Procedure:
In a 175-mL milk-dilution bottle fitted with a bakelite screw cap and a Teflon insert and rotated end-over-end at 20/min, (1) was equilibrated with an excess of (2) at 25±0.02 °C, sampled (5 mL±0.2%) with Hamilton syringes and titrated in an Aquatest II automatic Karl Fischer Titrator.

Source and Purity of Materials:
(1) Certified grade; washed successively with conc. H_2SO_4, H_2O, 1 N NaOH, H_2O, dried with silica gel, and distilled; d_4^{25} 0.87365
(2) Distilled.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: 0.00039 (std. dev.).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. B. Gramajo de Doz, C. M. Bonatti, N. Barnes, and H. N. Solimo, J. Chem. Thermodyn. **33**, 1663 (2001).

Variables:
One temperature: 303.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values
Solubility of benzene in water

T/K	g (1)/100 g sln	x_1 (compilers)
303.15	0.22	0.00051

Solubility of water in benzene

T/K	g (2)/100 g sln	x_2 (compilers)
303.15	0.04	0.0017

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Mixtures of known overall composition were prepared in 16 mL vials, intensively stirred for at least 7 days in a water bath and then allowed to settle for 24 h. Both phases were analyzed chromatographically (Hewlett Packard 6890 apparatus connected to a ChemStation HP G2070AA). The internal standard method was applied. Three or four analyses were performed for each sample.

Source and Purity of Materials:
(1) Merck, pure for analysis grade; purity checked by glc >99.8% mass %; used as received.
(2) Twice distilled.

Estimated Error:
Temperature: ±0.05 K.
Solubility: >1% (reproducibility).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. D. Gregory, S. D. Christian, and H. E. Affsprung, J. Phys. Chem. **71**, 2283 (1967).

Variables:
One temperature: 35 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in benzene at 35 °C was reported to be 0.0465 mol (2)/L sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0970 g (2)/100 g sln and $4.19 \cdot 10^{-3}$. The assumption that 1 L sln = 863 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
A solution of (2) in (1) was obtained using the solute isopiestic equilibrator described in Christian *et al.*[1] Water concentration was determined with a Beckman KF-3 aquameter by the Karl Fischer method.

Source and Purity of Materials:
(1) Source not specified, reagent grade; fractionally distilled using a 30-plate Oldershaw column.
(2) Not specified.

Estimated Error:
Temperature: ±0.05 °C.

References:
[1]S. D. Christian, H. E. Affsprung, J. R. Johnson, and D. Worley, J. Chem. Educ. **40**, 419 (1963).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Griswold, J. N. Chew, and M. E Klecka, Ind. Eng. Chem. **42**, 1246 (1950).

Variables:
Temperature: 25 °C and 50 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of benzene in water

t/°C	g (1)/100 g sln	$10^4 \cdot x_1$ (compiler)
25	0.18	4.2
50	0.22	5.5

Solubility of water in benzene

t/°C	g (2)/100 g sln	$10^4 x_2$ (compiler)
25	0.06	2.6
50	0.15	6.5

Auxiliary Information

Method/Apparatus/Procedure:
Samples of (1) or (2) were placed in glass-stoppered flasks mounted on a rotating shaft and immersed in a water bath.

Compositions were obtained by titrating a known sample, alternately adding the major and minor components from microburets until the two-phase point was found accurately. The flask was reimmersed in the bath after each titration to maintain thermal equilibrium. Finally, one drop of reagent would cause the second phase to appear or to disappear.

Source and Purity of Materials:
(1) Koppers Co.; industrial pure grade; purified by distillation with acetone and purity 99.07%.
(2) Distilled.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±0.1% (not specified).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. Groschuff, Z. Elektrochem. **17**, 348 (1911).

Variables:
Temperature: 3 °C–77 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of water in benzene

t/°C	x_2 (compiler)	g (2)/100 g sln
3	0.0013	0.030
23	0.0026	0.061
40	0.0049	0.114
55	0.0079	0.184
66	0.0110	0.255
77	0.0145	0.337

Auxiliary Information

Method/Apparatus/Procedure:
In 1 L long-necked flask (1) was placed and (2) was added dropwise.

Source and Purity of Materials:
(1) Kahlbaum; stored over Na; distilled twice from K-Na alloy; melting point 5.4 °C.
(2) Not specified.

Estimated Error:
Temperature: ±1 °C–2 °C.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

Variables:
One temperature: 30 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of benzene in water at 30 °C was reported to be 1.85 g (1)/kg(2) and 0.0237 mol (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.185 g (1)/100 g sln and $4.27 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
Saturated solutions were prepared by shaking in a thermostat and were analyzed by means of an interferometer. The instrument used was a combination liquid and gas interferometer made by Zeiss.

Source and Purity of Materials:
(1) Eastman Kodak Co., best grade; distilled; melting point 5.40 °C.
(2) Distilled.

Estimated Error:
Solubility: 1.0% (from values of duplicate determinations).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).

Variables:
Temperature: 153 °C–254 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values
Solubility of benzene in water

t/°C	$10^3 \cdot x_1$ (compiler)	g (1)/100 g sln
153	2.978	1.283
178	5.044	1.913
204	6.844	2.902
225	9.000	3.790
241	10.67	4.471
254	12.17	5.073

Auxiliary Information

Method/Apparatus/Procedure:
The measurements were made in sealed glass tubes. No more details were reported in the paper.

Source and Purity of Materials:
(1) Source not specified; n_D^{20} 1.5011.
(2) Doubly distilled.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. Hayashi and T. Sasaki, Bull. Chem. Soc. Jpn. **29**, 857 (1956).

Variables:
Temperature: 20 °C and 25 °C

Prepared By:
A. Maczynski

Experimental Values
Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln
20	3.16	0.137
25	4.16	0.180

Auxiliary Information

Method/Apparatus/Procedure:
The experiment has been described for the determination of the solubility in a ternary system (1)–(2)-Tween 80.

Source and Purity of Materials:
(1) Source not specified; shaken repeatedly with concentrated H_2SO_4, boiled with H_2O, recrystallized several times and distilled over Na metal.
(2) Not specified.

Estimated Error:
Solubility: more than 0.4 g (1)/100 g sln (type of error not specified).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. Herz, Ber. Dtsch. Chem. Ges. **31**, 2669 (1898).

Variables:
One temperature: 22 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of benzene in water at 22 °C was reported to be 0.082 mL (1)/100 mL (2).

Auxiliary Information

Method/Apparatus/Procedure:
The composition of the saturated solution was evaluated by extrapolation of calibration density measurements (carried out on a series of synthetic solutions) to the measured density of the solution. The maximum difference between the actual and the synthetic densities was a few units in the third decimal place.

Source and Purity of Materials:
(1) Not specified.
(2) d^{22} 0.9980 g/mL.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. E. Hill, J. Am. Chem. Soc. **44**, 1163 (1922).

Variables:
One temperature: 0 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 0 °C was reported to be 0.153 g (1)/100 g sln.
The corresponding mole fraction, x_1, calculated by compiler is $3.53 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
Three determinations of freezing point of (2) saturated with (1) gave 0.037 °C as the average depression.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. E. Hill, J. Am. Chem. Soc. **45**, 1143 (1923).

Variables:
Temperature: 5.4 °C–69.5 °C

Prepared By:
A. Maczynski and A. Maczynska

Experimental Values

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
5.4[a]	1.5	0.034
15.0	2.3	0.054
25.0	3.2	0.073
37.5	5.2	0.115
50.0	6.7	0.156
57.5	8.0	0.185
65.0	9.9	0.230
69.5[b]	11.4	0.265

[a]Quadruple point.
[b]Boiling point of 2-liquid system.

Author's smoothing equation: $S = 0.03294 + 0.0006449 \cdot t + 0.00003728 \cdot t^2$ where $S = g$ (2)/100 g sln

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was mechanically stirred at various temperatures and, after saturation was obtained, was transferred to small cylinders, treated with weighed amounts of silver perchlorate and the solubility of the salt in the mixed solvent determined at 25 °C. After a correction for the amount of (1) present in the solid phase, the original (2) content of the saturated solution could be determined from the reference curve.

Source and Purity of Materials:
(1) Source not specified; purified by recrystallization; dried over calcium chloride and finally over bright sodium wire; melting point 54 °C or higher.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in benzene was reported to be 0.032 mol (2)/L sln at 25 °C.

The corresponding mass percent and mol fraction, x_2, calculated by the compilers are 0.066 g (2)/100 g sln and $2.9 \cdot 10^{-3}$. The assumption that 1 L sln = 874 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
The water determination was carried out according to Johansson's modification of the Karl Fischer titration in Hardy *et al.*[1] and Johansson.[2]

Source and Purity of Materials:
(1) Source not specified, 0.04% of toluene; purity 99.6%; used as received.
(2) Not specified.

Estimated Error:
Temperature: ±0.3 °C.
Solubility: ±0.001 mol (2)/L sln (type of error not specified).

References:
[1]C. J. Hardy, B. F. Greenfield, and D. Scargill, J Chem. Soc. **90** (1961).
[2]A. Johansson, Sv. Papperstidn. 11B, **124** (1947).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Jäger, Brennst.-Chem. **4**, 259 (1923).

Variables:
Temperature: 100 °C–300 °C

Prepared By:
A. Maczynski

Experimental Values
Solubility of benzene in water

t/°C	mL (1)/100 mL (2)
100	0.2
150	0.6
200	2.1
250	7.3
285	10.6
300	14.6

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined in sealed glass tubes.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error: Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. Janado, Y. Yano, Y. Doi, and H. Sakamoto, J. Solution Chem. **12**, 741 (1983).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values
Solubility of benzene in water

t/°C	mg (1)/L (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	1811	0.1813	$4.187 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. About 10 g of water with an excess of benzene was placed in a thermostat, stirred for 6 h gently shaken for another 18 h, and next allowed to stand for separation for next 6 h. A portion of a clear solution was placed in a 15 mL vial containing a weighed amount of *n*-hexane. After extracting into *n*-hexane, benzene was determined by spectrophotometry.

Source and Purity of Materials:
(1) Nakarai Chemicals Ltd.; analytical grade; used as received.
(2) Glass redistilled water.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: <1.0% (average deviation from the mean).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. R. Johnson, S. D. Christian, and H. E. Affsprung, J. Chem. Soc. A 77 (1966).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in benzene at 25 °C was reported to be 0.0349 mol (2)/L sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0719 g (2)/100 g sln and $3.11 \cdot 10^{-3}$. The compiler's calculation assumes a solution density of 1.00 g·/mL.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus described in Christian *et al.*[1] was used without modification. Samples were equilibrated in a constant-temperature water-bath maintained at 25±0.1 °C. Water solubility was determined by using a Beckman Model KF-3 Aquameter.

Source and Purity of Materials:
(1) Source not specified; certified or reagent grade; distilled through a 30-plate Oldershaw column.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±0.0005 mol(2)/L sln (type of error not specified).

References:
[1]S. D. Christian, H. E. Affsprung, J. R. Johnson, and J. D. Worley, J. Chem. Educ. **40**, 419 (1963).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. R. Jones and C. B. Monk, J. Chem. Soc. 2633 (1963).

Variables:
Temperature: 25 °C–35 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

Solubility of water in benzene

t/°C	$10^4 \cdot$ mL(2)/mL(1)
25	5.7
30	6.5
35	7.5

Auxiliary Information

Method/Apparatus/Procedure:
In a thermostatted glass-stoppered flask 10–25 mL (1) was shaken for a minimum 4 h with titrated water (a few mL of HTO equivalent to ~2 mCi/mL) and decanted. A 5-mL aliquot was reshaken for 4 h with 5 mL H_2O in a 10-mL flask, sampled and assayed with a Nuclear Enterprises type 8301 liquid scintillation counter. The two-stage process eliminates quenching effects (due to solvent) on the scintillator.

Source and Purity of Materials:
(1) Analar grade repurified by conventional methods.[1]
(2) Not specified.

Estimated Error:
Solubility: 5%±1% (average deviation).

References:
[1]Vogel, *Practical Organic Chemistry* (Longmans, Green and Co., London, 1956).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. Karisson, J. Chem. Eng. Data **18**, 290 (1973).

Variables:
Temperature: 14 °C–35 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

Solubility of benzene in water

t/°C	$10^3 \cdot x_2$ (compiler)	$10^2 \cdot g$ (2)/100 g sln (compiler)	mg (2)/kg (1)
14.97	2.31	5.33	533.0
17.94	2.56	5.91	591.3
20.05	3.74	6.31	631.4
22.95	2.98	6.87	686.7
24.90	3.14	7.24	724.8
27.97	3.14	8.03	803.2
29.95	3.70	8.53	853.5
31.96	3.97	9.16	915.8
35.06	4.43	10.21	1021.1

Auxiliary Information

Method/Apparatus/Procedure:
The determination of the solubility of (2) in (1) was based on an accurate method for determining small amounts of water via coulometrically generated iodine at a controlled potential by the Karl Fischer method as described in Karisson[1] and Karisson and Karrman.[2] Two 100-mL Erlenmeyer flasks, each containing 10 mL of (2) and 40 mL of (1), were placed in a water bath. The temperatures were measured with a platinum resistance thermometer. When equilibrium was reached, samples were withdrawn from the benzene phase with a dried Agla microsyringe and immediately added through a membrane to the electrolysis cell.

Source and Purity of Materials:
(1) Fisher Scientific Co., thiophene-free; twice recrystallized.
(2) Twice distilled.

Estimated Error:
Temperature: ±0.3 °C.
Solubility: ±0.3% (type of error not specified).

References:
[1]R. Karisson, Talanta **19**, 1639 (1972).
[2]R. Karisson and K. J. Karrman, Talanta **18**, 459 (1951).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **33**, 87 (1988).

Variables:
One temperature 25.00 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

t/°C	mol (1)/L sln	g (1)100 g sln (compilers)	x_1
25.00	$2.17 \cdot 10^{-2}$	0.1693	$3.91 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were determined by headspace chromatographic analysis, Keeley and Meriwether,[1] using a multiple injection interrupted flow technique. Samples were prepared in septum bottles of 160 mL volume which were thermostated and shaken for 72 h prior to analysis. For analysis each bottle was transferred to a tempering beaker and pressurized to 15.00 psig with chromatographic grade nitrogen. Bottles were attached to the headspace sampling port of a gas chromatograph with a flame ionization detector. Solubility was calculated on the basis of Henry's law.

Source and Purity of Materials:
(1) Baker Instra; analyzed grade; purity 99.97% by glc.
(2) Deionized water.

Estimated Error:
Temperature: ±0.01 °C.

References:
[1]D. F. Keeley and J. R. Meriwether, Rev. Sci. Instrum. **75**, 1434 (1986).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Kirchnerova and G. C. B. Cave, Can. J. Chem. **54**, 3909 (1976).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in benzene at 25 °C was reported to be 0.0349 mol (2)/L sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0719 g (2)/100 g sln and $3.11 \cdot 10^{-3}$. The assumption that 1 L sln = 874 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 50 mL of (1) was placed in the equilibration vessel. A test tube containing 6 mL of (2) was then placed in the vessel so that the rim of the test tube rested against the upper inside wall of the vessel. The vessel was stoppered, placed inside a plastic bag, and the jacketed vessel was submerged up to its neck in a water thermostat. Trials had shown that the concentration of (1) in (2) became constant within 2 days. The concentration of water was determined by a conventional Karl Fischer deadstop back-titration.

Source and Purity of Materials:
(1) Fisher B-245; purified by double crystallization; d_4^{25} 0.87378.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 0.0002 mol (2)/L sln (standard deviation from 5 determinations).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).

Variables:
Temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 1.86 g (1)/L sln and 0.0239 mol (1)/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.186 g (1)/100 g sln and $4.31 \cdot 10^{-4}$. The assumption that 1.00 L sln = 1.00 kg sln was used in this calculation.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectrophotometry.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. M. Korenman and R. P. Aref'eva, Zh. Prikl. Khim. (Leningrad) **51**, 957 (1978).

Variables:
Temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 0.82 g (1)·/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.084 g (1)/100 g sln and $1.94 \cdot 10^{-4}$. The compiler's calculation assumes a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:
About 200–500 mL (2) was placed in a ground-joint glass cylinder and 20–50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks were made to determine the excess of (1).

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Solubility: 0.01 g (1)/L sln (standard deviation from 6 determinations).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. Ya. Krasnoshchekova and M. Ya. Gubergrits, Vodnye Resursy **2**, 170 (1975).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 1.000 mg (1)/mL sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 100 mg (1)/100 g sln and $2.305 \cdot 10^{-4}$. The compiler's calculation assumes a solution density of 1.000 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by glc. A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90 °C–140 °C.

Source and Purity of Materials:
(1) Described in Krasnoshchekova and Gubergrits.[1]
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.

References:
[1]P. Ya. Krasnoshchekova and M. Ya. Gubergrits, Neftekhimiya **13**, 885 (1973).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [732-18-5]

Original Measurements:
A. P. Kudchadker and J. J. McKetta, Pet. Refin. **41**, 191 (1962).

Variables:
Temperature: 37.8 °C–137.8 °C
Pressure: 0.1 MPa–5.7 MPa

Prepared By:
A. Maczynski

Experimental Values

Solubility of benzene in water

t/°F	t/°C (compiler)	$10^4 \cdot x_1$	g (1)/100 g sln (compiler)	P/psia	P/MPa (compiler)
100	37.8	1.24	0.0538	15.8	0.109
		1.32	0.0572	20.2	0.139
		1.57	0.0681	37.9	0.261
		1.66	0.0720	49.2	0.339
		2.06	0.0893	97.1	0.669
		2.61	0.113	161.35	1.112
		3.28	0.142	225.7	1.556
		3.43	0.149	244.2	1.684
		4.01	0.174	308.2	2.125
		4.84	0.201	373.7	2.577
		4.98	0.216	406.3	2.801
		5.78	0.250	486.4	3.354
		6.41	0.277	554.8	3.825
		6.84	0.296	635.2	4.380
		7.87	0.340	743.23	5.124
		8.5	0.38	822.7	5.672
160	71.1	1.75	0.0758	19.8	0.137
		1.91	0.0828	17.7	0.122
		1.88	0.0815	23.8	0.164
		2.01	0.0871	27.5	0.190
		2.24	0.0971	37.6	0.259
		2.81	0.1218	74.0	0.510
		4.80	0.2078	209.8	1.447
		5.71	0.2471	260.2	1.794
		6.39	0.2765	314.3	2.167
		7.69	0.3327	390.6	2.693
		8.58	0.3710	449.1	3.096
		10.00	0.4326	509.8	3.536
		12.23	0.5283	607.2	4.186
220	104.4	2.35	0.1018	29.4	0.203
		2.93	0.1270	36.25	0.250
		3.50	0.1516	46.2	0.319
		3.80	0.1646	49.9	0.344
		4.89	0.2127	84.8	0.585
		7.68	0.332	165.2	1.139
		8.49	0.367	195.0	1.344
		9.39	0.406	204.6	1.411
		9.40	0.406	218.2	1.504
		10.75	0.465	259.3	1.788
		11.62	0.502	283.1	1.952
		13.28	0.573	327.8	2.260
		14.68	0.633	372.6	2.569
		16.85	0.727	447.5	3.085
		21.49	0.925	548.2	3.780
280	137.8	3.92	0.170	61.3	0.423
		5.84	0.253	76.2	0.525
		6.10	0.264	78.5	0.541
		7.78	0.337	103.7	0.715
		8.11	0.351	112.0	0.772
		8.28	0.358	114.9	0.792
		9.0	0.389	137.5	0.948
		10.55	0.456	170.0	1.172
		11.59	0.501	195.2	1.346
		14.28	0.616	265.1	1.766
		16.22	0.700	316.2	2.180
		16.98	0.732	325.1	2.241
		18.39	0.793	356.2	2.456
		20.20	0.870	402.6	2.776
		23.0	0.990	462.5	3.189

Author's smoothed values

t/°C (compiler)	$10^4 \cdot x_1$	P/psia
37.8	1.18	14.7
71.1	1.56	14.7
37.8	1.33	20.0
71.1	1.80	20.0
104.4	1.01	20.0
37.8	1.58	40.0
71.1	2.22	40.0
104.4	3.16	40.0
37.8	1.75	60.0
71.1	2.58	60.0
104.4	4.16	60.0
137.8	3.52	60.0
37.8	1.92	80.0
71.1	2.89	80.0
104.4	4.88	80.0
137.8	6.20	80.0
37.8	2.10	100.0
71.1	3.17	100.0
104.4	5.61	100.0
137.8	7.53	100.0
37.8	2.58	150.0
71.1	3.89	150.0
104.4	7.18	150.0
137.8	9.71	150.0
37.8	3.03	200.0
71.1	4.60	200.0
104.4	8.61	200.0
137.8	11.82	200.0
37.8	3.50	250.0
71.1	5.52	250.0
104.4	10.61	250.0
137.8	13.74	250.0
37.8	3.98	300.0
71.1	6.24	300.0

104.4	12.32	300.0
137.8	15.80	300.0
37.8	4.41	350.0
71.1	7.20	350.0
104.4	14.03	350.0
137.8	17.84	350.0
37.8	4.85	400.0
71.1	8.15	400.0
104.4	15.80	400.0
137.8	20.00	400.0
37.8	5.30	450.0
71.1	9.05	450.0
104.4	17.61	450.0
137.8	22.38	450.0
37.8	5.77	500.0
71.1	10.00	500.0
104.4	19.56	500.0
37.8	6.21	550.0
71.1	11.06	550.0
104.4	21.54	550.0
37.8	6.68	600.0
71.1	12.01	600.0
37.8	7.13	650.0
37.8	7.54	700.0
37.8	7.94	750.0
37.8	8.35	800.0

Author's smoothed values calculated by compiler

t/°C	g (1)/100 g sln	P/MPa
37.8	0.0512	0.101
71.1	0.0676	0.101
104.4	—	0.101
137.8	—	0.101
37.8	0.0577	0.138
71.1	0.0780	0.138
104.4	0.0438	0.138
137.8	—	0.138
37.8	0.0685	0.276
71.1	0.0962	0.276
104.4	0.1369	0.276
137.8	—	0.276
37.8	0.0758	0.414
71.1	0.1109	0.414
104.4	0.1802	0.414
137.8	0.1525	0.414
37.8	0.0832	0.552
71.1	0.1252	0.552
104.4	0.2113	0.552
137.8	0.2683	0.552
37.8	0.0910	0.689
71.1	0.1373	0.689
104.4	0.2428	0.689
137.8	0.3258	0.689
37.8	0.1118	1.034
71.1	0.1685	1.034
104.4	0.3107	1.034
137.8	0.4198	1.034
37.8	0.1313	1.379
71.1	0.1992	1.379
104.4	0.3723	1.379
137.8	0.5106	1.379
37.8	0.1516	1.724
71.1	0.2390	1.724
104.4	0.4585	1.724
137.8	0.5975	1.724
37.8	0.1724	2.068
71.1	0.2701	2.068
104.4	0.5321	2.068
137.8	0.6817	2.068
37.8	0.1910	2.413
71.1	0.3115	2.413
104.4	0.6057	2.413
137.8	0.7691	2.413
37.8	0.2100	2.758
71.1	0.3525	2.758
104.4	0.6817	2.758
137.8	0.8615	2.758
37.8	0.2290	3.103
71.1	0.3913	3.103
104.4	0.7593	3.103
137.8	0.9634	3.103
37.8	0.2500	3.447
71.1	0.4323	3.447
104.4	0.8428	3.447
137.8	—	3.447
37.8	0.2690	3.792
71.1	0.4779	3.792
104.4	0.9275	3.792
137.8	—	3.792
37.8	0.2890	4.137
71.1	0.5188	4.137
104.4	—	4.137
137.8	—	4.137
37.8	0.3080	4.482
71.1	—	4.482
104.4	—	4.482
137.8	—	4.482
37.8	0.3260	4.826
71.1	—	4.826
104.4	—	4.826
137.8	—	4.826
37.8	0.3430	5.171
71.1	—	5.171
104.4	—	5.171
137.8	—	5.171
37.8	0.3610	5.551
71.1	—	5.551
104.4	—	5.551
137.8	—	5.551

Auxiliary Information

Method/Apparatus/Procedure:

The experimental apparatus and analytical technique are described in Davis.[1] The equilibrium apparatus consisted of a jacketed cell with an internal heating coil. The mixing of the contents of the cell was achieved by a rocking mechanism.

Source and Purity of Materials:

(1) Phillips Petroleum Co., purity 99.0 mole %; used as received.
(2) Distilled and boiled to remove any dissolved gases.

Estimated Error:

Not specified.

References:

[1]J. E. Davis, The Solubility of Methane and Ethylene in Water, M. S. Thesis, the University of Texas, Austin, Texas, 1959.

Components:

(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. **51**, 230 (1973).

Variables:

One temperature: 25 °C

Prepared By:

A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 1765 mg (1)/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.1765 g (1)/100 g sln and $4.07 \cdot 10^{-4}$. The compiler's calculation assumes a solution density of 1.000 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was equilibrated at 25 ± 0.1 °C for a minimum of 12 h in a 200-mL Teflon-stoppered vessel (25 cm long and 3.5 cm across) with gentle shaking, allowed to settle for 6 h and tested for the absence of emulsion (Tyndall effect). The aqueous and organic phases were analyzed by glc with internal standarization) on a Hewlett-Packard Model 700 instrument equipped with a 15% SE-30 on 60/80 mesh acid-washed $(CH_3)_2Cl_2Si$-treated Chromosorb P column (steel capillary 10 ft × 0.125 inch). The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analyzed by glc.

Source and Purity of Materials:

(1) Phillip Petroleum Co. research grade, 99+ mole %; used as received.
(2) Doubly distilled.

Estimated Error:

Temperature: ± 0.1 °C.
Solubility: 30 mg (1)/L (2 std. dev.).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. M. Lo, C. L. Tseng, and J. Y. Yang, Anal. Chem. **58**, 1596 (1986).

Variables:
One temperature: 25 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

t/°C	g (1)/100 g sln	x_1 (compilers)
25	0.181 ± 0.015	$4.18 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
The radiometric method was used. The radioagent $^{60}Co(PDC)_3$ was first dissolved in component (1) before pure water was added. Both of the liquids were placed in a 1000-mL separatory funnel. The mixture was shaken for 5 min and allowed to separate for next 30 min. Concentration was calculated from activity measurements by a NaI(Tl) scintillation detector.

Source and Purity of Materials:
(1) E. Merck; purity not specified.
(2) Demineralized and degassed.

Estimated Error:
Solubility: as above (standard deviation of the mean).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. **53**, 239 (1975).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 1.7795 g (1)/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.178 g (1)/100 g sln and $4.11 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility of (1) in (2) was determined by gas chromatography. The gas chromatograph was Hewlett-Packard Model 5750 equipped with a hydrogen flame ionization detector. Many details were given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Co., research grade; 99.9+%; used as received.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±0.0164 g (1)/L sln.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. L. Masterton and M. C. Gendrano, J. Phys. Chem. **70**, 2895 (1966).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in benzene at 25 °C was reported to be 0.0347 mol (2)/L sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0715 g (2)/100 and $3.09 \cdot 10^{-3}$. The assumption that 1 L sln = 874 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
Equilibration of (1) and (2) was allowed to take place for at least 2 days. The organic phase was analyzed for water by the Karl Fischer method.

Source and Purity of Materials:
(1) Source not specified; free from thiophene; used as received.
(2) Not specified.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: 0.0002 mol (2)/L (mean deviation from duplicate determinations).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 997 (1978).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 1791 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, values calculated by compiler are 0.1791 g (1)/100 g sln and $4.130 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
The dynamic coupled liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in May *et al.*[1]

Source and Purity of Materials:
(1) Commercial product; less than 3% impurities.
(2) Distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa)

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±10 mg(1)/100 kg(2) (std. dev.).

References:
[1]W. May, S. Chesler, Cram, B. Gump, H. Hertz, D. Enagonio, and S. Dyszel, J. Chromatogr. Sci. **13**, 535 (1975).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. E. May, S. P. Wasik, M. M. Miller, Y. B. Tewari, J. M. Brown-Thomas, and R. N. Goldberg, J. Chem. Eng. Data **28**, 197 (1983).

Variables:
Temperatures: 273.35 K–298.95 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

T/K	g (1)/100 g sln (compilers)	$10^4 \cdot x_1$
273.35	0.18323	4.232
279.35	0.18008	4.159
284.15	0.17956	4.147
287.15	0.17666	4.080
290.05	0.17588	4.062
291.75	0.17636	4.073
298.15	0.17878	4.129
298.95	0.18155	4.193

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by an automated coupled-column liquid chromatographic apparatus; the technique and apparatus were reported in May *et al.*[1] and Tewari *et al.*[2] A saturated solution was generated by pumping water through a column containing the solute coated on Chromosorb W. The HPLC method and UV detection were used for analysis.

Source and Purity of Materials:
(1) Source not specified; purity>99 mole % by glc.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 K (Tewari *et al.*[2]).

References:
[1]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[2]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 0.1780 g (1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compilers is $4.11 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was injected directly into a gas liquid chromatograph.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; 99+%; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 0.0045 (standard deviation of mean).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. W. McBain and K. J. Lissant, J. Phys. Colloid Chem. **55**, 665 (1951).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson and G. T. Hefter

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 0.151 g (1)/100 mL sln.

The corresponding mass percent and mole fraction solubility, calculated by the compilers assuming a solution density of 1.00 kg/L, are 0.151 g (1)/100 g sln and $x_1 = 3.48 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
10 mL portions of (2) were pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the amount solubilized.

Source and Purity of Materials:
(1) C.P. grade.
(2) Distilled and boiled to remove CO_2.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454 (1953).

Variables:
One temperature: 100 °F

Prepared By:
G. T. Hefter

Experimental Values

The solubility of benzene in water at 100 °F (311 K) was reported to be 0.5 g (1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compiler, is $1.2 \cdot 10^{-3}$.

The solubility of water in benzene at 100 °F (311 K) was reported to be <0.3 g (2)/100 g sln.

The corresponding mole fraction, x_2, calculated by the compiler, is $<1.3 \cdot 10^{-2}$.

Auxiliary Information

Method/Apparatus/Procedure:
The method was essentially that of Washburn *et al.*[1] and involved titration of the second component to the cloud point, in a constant temperature bath.

Source and Purity of Materials:
(1) Baker; thiophene free; used without further purification; n_D^{20} 1.5004.
(2) Distilled.

Estimated Error:
Not specified.

References:
[1]E. R. Washburn, V. Hnizda, and R. D. Vold, J. Am. Chem. Soc. **53**, 3232 (1931).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. F. McDevit and F. A. Long, J. Am. Chem. Soc. **74**, 1773 (1952).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 1.775 mol (1)/L sln. Presumably this should be 1.775 g (1)/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler assuming a solution density of 1.000 g/mL are 0.1775 g (1)/100 g sln and $4.091 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by a variation of the Euler method in which a measured excess volume of (1) is added to (2). After equilibration, the volume of undissolved (1) is determined by measuring its length in a precision bore tube which leads from the top of the apparatus.

Source and Purity of Materials:
(1) Source not specified, reagent grade; thiophene-free; distilled; purity not specified.
(2) Doubly distilled.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: ±0.5% (from duplicate determinations).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).

Variables:
Temperature: 298.0 K–473.0 K
Pressure: 1 bar–400 bar

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

T/K	P/bar	g (1)/100 g sln (compilers)	$10^3 \cdot x_1$
298.0	1	0.00173	0.40±0.01
298.0	65	0.00173	0.40±0.02
298.0	400	0.00143	0.33±0.01
323.0	65	0.00203	0.47±0.03
373.0	65	0.00385	0.89±0.06
423.0	65	0.00947	2.2±0.2
473.0	65	0.0213	5.0±0.3
473.0	400	0.0175	4.1±0.3

Auxiliary Information

Method/Apparatus/Procedure:
The dynamic method described in Miller and Hawthorne[1] was used. The high-pressure saturation cell was filled with component (1) and placed in the oven of gas chromatograph to provide precise temperature control. Next water was pumped into the saturation cell. After a 60 min equilibration 10 fractions were collected for 3 min each. The details of filling procedure, equilibration, and sampling were described in the paper. The analyses were performed using an HP model 5890 gas chromatograph with flame ionization detection.

Source and Purity of Materials:
(1) Sigma-Aldrich, Milwaukee, WI.; purity>99%; used as received.
(2) Not stated.

Estimated Error:
Temperature: ±0.1 K.
Solubility: as above.

References:
[1]D. J. Miller and S. B. Hawthorne, Anal. Chem. **70**, 1618 (1998).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. H. Milligan, J. Phys. Chem. **28**, 494 (1924).

Variables:
One temperature: 25 °C

Prepared By:
G. T. Hefter

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 0.07 mL (1)/100 ml (2).

Auxiliary Information

Method/Apparatus/Procedure:
20 mL of benzene/air vapor were introduced into a glass cell, containing 120 mL of air-saturated distilled water in a thermostatted water bath. The apparatus was removed from the bath and shaken for 2 min to bring about equilibrium. Benzene solubility in water was determined by analysis of the vapor by combustion in a Haldane apparatus before and after equilibration.

Source and Purity of Materials:
(1) Not specified.
(2) Distilled.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and F. Billett, J. Chem. Soc. 3819 (1952).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 0.0220 mol(1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by compilers are 0.172 g (1)/100 g sln and $x_1 = 3.96 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
After an excess of (1) had been shaken with about 1 L of (2) for about 1 week, a known volume of saturated solution was made slightly alkaline, and a stream of pure air passed through to drive off (1). After passage through a silica tube packed with cupric oxide and heated to redness, the (2) was removed by concentrated sulfuric acid and calcium chloride and the carbon dioxide absorbed and weighed in soda-asbestos. The precautions usual in organic combustion were taken.

Source and Purity of Materials:
(1) Source not specified; purest obtainable material; distilled; purity not specified.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±0.5% (mean of large numbers of determinations).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. C. Moule and W. Thurston, Can. J. Chem. **44**, 1361 (1966).

Variables:
Temperature: 9.44 °C–49.45 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of water in benzene

t/°C	$10^3 x_2$ (compiler)	g (2)/100 g sln (compiler)	mg (2)/kg (1)
9.44	1.92	0.0443	442.5
14.98	2.30	0.0530	530.2
20.10	2.77	0.0639	639.2
24.54	3.14	0.0726	726.0
29.52	3.67	0.0848	848.0
34.88	4.40	0.102	1017.1
40.06	5.09	0.117	1177.8
43.78	5.76	0.133	1333.7
49.45	6.78	0.157	1570.6

Auxiliary Information

Method/Apparatus/Procedure:
A method based on an isotope dilution procedure was used. This method involves the exchange of the water present in the sample with D_2O determined by infrared difference spectroscopy.

Source and Purity of Materials:
(1) Fisher Certified reagent grade; distilled twice and dried over molecular sieve (Linde No. 4A).
(2) From Ottawa River (0.0146 mole % D_2O; distilled from alkaline permanganate).

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±0.8% (mean of three determinations).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Niini, Suom. Kemistil. A **2**, 19 (1938).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 20 °C was reported to be 0.085 g (1)/100 g sln.
The corresponding mole fraction, x_1, calculated by compiler is $2.0 \cdot 10^{-4}$.
The solubility of water in benzene at 20 °C was reported to be 0.059 g (2)/100 g sln.
The corresponding mole fraction, x_2, calculated by compiler is $2.6 \cdot 10^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
The weight concentration was determined by combined refractometry and pycnometry.

Source and Purity of Materials:
(1) Kahlbaum; analytical grade; dried with P_2O_5 and distilled; purity not specified.
(2) Not specified.

Estimated Error:
Solubility: ±0.005 g (2)/100 g sln (type of error not specified).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. M. O'Grady, J. Chem. Eng. Data **12**, 9 (1967).

Variables:
Temperature: 288 °C and 293 °C
Pressure: 3600 psig (24.9 MPa)

Prepared By:
A. Maczynski

Experimental Values

Solubility of benzene in water

t/°C	x_1 (compiler)	g (1)/100 g sln	P/psig	P/MPa (compiler)
288	0.0513	19.0	3600	24.9
293	0.0751	26.3	3600	24.9

Solubility of water in benzene

t/°C	x_2 (compiler)	g (2)/100 g sln	P/psig	P/MPa (compiler)
288	0.677	32.6	3600	24.9
293	0.751	41.0	3600	24.9

Auxiliary Information

Method/Apparatus/Procedure:
Measured amounts of (1) and (2) of known composition were pumped into the extractor and mixed for 1 or 2 h. The phases were allowed to settle for about 2 h; then the contents were slowly (1.5 mL/min) displaced at constant pressure with mercury. The product was collected in 2–5 mL cuts in burets with 0.1 mL subdivisions. The (1)–(2) composition could be read directly.

Source and Purity of Materials:
(1) Phillips research grade; less than 0.2% impurities; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±0.1 °C.
Pressure: ±10 psi.
Solubility: ±0.02 mL (2).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. A. Pavia, Thesis, North Carolina State College, Raleigh, N.C., U.S.A, 1958.

Variables:
Temperature: 9.3 °C–65 °C

Prepared By:
C. Tsonopoulos and G. T. Hefter

Experimental Values

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln[a]	P_1^s/mm Hg
9.28	1.783	0.04117	8.774
20.00	2.592	0.05989	17.535
20.00	2.629	0.06076	17.535
30.17	3.597	0.08318	32.136
40.15	4.845	0.11216	55.764
49.97	6.567	0.15222	92.37
59.90	8.657	0.2010	148.70
65.00	9.730	0.2261	187.54

[a]Average of three separate analysis.

Results were represented with a "probable deviation of 0.8%" by the equation

$$\log_{10}(100s) = 0.117135 + 0.5162095 \log_{10} P_1^s + 0.0127866(\log_{10} P_1^s)^2,$$

where s is the solubility of water in benzene in g (2)/100 g sln and P_1^s is the equilibrium vapor pressure of the solution.

Auxiliary Information

Method/Apparatus/Procedure:
Water and benzene were equilibrated in a 4-L pyrex vessel fitted with a stirrer. Equilibration typically required about 100 h of stirring. Care was taken to avoid condensation of water on the vessel lid and selective absorption of water on the glass walls. Samples of analysis were withdrawn by air pressure. Water was determined by the Karl Fischer titration.

Source and Purity of Materials:
(1) Distilled in a tinned Barnstead still [specific conductivity $(5-20)\cdot 10^{-7}\cdot \omega^{-1}$].
(2) Allied Chemical: purified by triple fractional crystallization; purity 99.99 mol%; n (D, 25 °C) 1.49806.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: ±1% relative; type of error not stated

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).

Variables:
Temperature: 278.26 K–318.36 K

Prepared By:
M. C. Haulait-Pirson

Experimental Values
Solubility of benzene in water

T/K	$10^3 \cdot x_1$	g (1)/100 g sln
278.26	0.4776	0.2071 ± 0.0052
288.06	0.4792	0.2078 ± 0.0055
293.06	0.4809	0.2085 ± 0.0040
298.16	0.4815	0.2088 ± 0.0038
308.26	0.4848	0.2102 ± 0.0046
318.86	0.5304	0.2300 ± 0.0054

Auxiliary Information

Method/Apparatus/Procedure:
10 mL of (2) were placed along with 4–10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in a rotating basket and rotated for 24 h. The bottles were then hand shaken to remove (1) droplets from the stoppers and replaced in a bath with the tops down for an additional 24 h. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions, and calculation are given in the paper.

Source and Purity of Materials:
(1) Matheson, Coleman & Bell; Chromatoquality; 99+ mole%; used as received.
(2) Laboratory distilled water.

Estimated Error:
Solubility: standard deviation, at least from 15 measurements, is given above.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Variables:
Temperature: 0 °C–25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values
Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln (compiler)	mg (1)/kg (2)
0[†a]	3.87	0.167	1678[c]
25[b]	4.05	0.175	1755[c]

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln (compiler)	mg (2)/kg (1)
0[‡a]	1.31	0.030	302[d]
25[b]	2.99	0.069	692[e]

[†]Benzene was at supercooled liquid state.
[‡]Solubility in supercooled liquid.
[a–e]see Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.
The solubility of water in the organic layer was determined by the Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:
Temperature: (a) ±0.02 °C, (b) ±0.01 °C.
Solubility: (c) ±1.7%, (d) ±4.7%, (e) ±3.1% (from two or three determinations).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

The solubility of benzene in water at 25 °C and at system pressure was reported to be 1740 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.174 g (1)/100 g sln and 4.01×10^{-4}.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined at laboratory temperature by use of screw-cap test tubes. The (1) phase floated on top of the water and ensured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.
Solubility: ±17 mg (1)/kg (2).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. J. Rebert and W. B. Kay, AIChE J. **5**, 285 (1959).

Variables:
Temperature: 282.8 °C–306.4 °C
Pressure: 11.51 MPa–15.87 MPa

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

Solubility of benzene in water

t/°C	x_1 (compiler)	g (1)/100 g sln	P/psia	P/MPa (compiler)
287.5	0.030	11.7	1763	12.16
301.7	0.061	22	2118	14.60
306.4	0.111	35.1	2301	15.86
306.4*	0.138	41	2302	15.87

Solubilityofwater inbenzene

t/°C	x_2 (compiler)	g (2)/100 g sln	P/psia	P/MPa (compiler)
282.8	0.649	29.9	1670	11.51
297.5	0.667	31.6	1992	13.73
306	0.818	50.9	2302	15.87
306.4[a]	0.862	59	2302	15.87

[a]Upper critical solution temperature.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus employed was a modification of that described in Young[1] and Kay[2] for P-T-x studies. A schematic diagram and construction details amply reported.

Source and Purity of Materials:
(1) Source not specified, reagent grade; dried over P_2O_5 and distilled; purity not specified.
(2) Freshly prepared, conductivity grade.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±0.022 wt. fraction.
Pressure: ±1 lb/in.

References:
[1]S. Young, *Stoichiometry Longmans* (Green, New York, 1918), p. 122.
[2]W. B. Kay, Ind. Eng. Chem. **30**, 450 (1938).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. B. Robertson, S. Afr. J. Sci. **30**, 187 (1933).

Variables:
One temperature: 5.4 °C

Prepared By:
G. T. Hefter

Experimental Values

The solubility of water in benzene at 5.4 °C was reported to be 0.035%, corresponding to 0.035 g (2)/100 g sln.

The corresponding mole fraction (x_2), calculated by the compiler, is 1.5×10^{-3}.

Auxiliary Information

Method/Apparatus/Procedure:
Moist benzene-saturated air was allowed to bubble through moist benzene in a freezing-point tube until a constant freezing point was obtained. A few drops of distilled water were then added and the solution stirred for some time and the freezing point redetermined. The water content of the saturated sln was calculated from the freezing point depression (relative to pure benzene) by assuming the water to be monomolecular in solution.

Source and Purity of Materials:
(1) Kahlbaum, pro-analysis, used without further purification.
(2) Distilled, purity not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. W. Roddy and C. F. Coleman, Talanta **15**, 1281 (1968).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in benzene at 25 °C was reported to be $x_2=3.23\times10^{-3}$ and 0.0363 mol (2)/L sln.

The corresponding mass percent value calculated by the compilers is 0.0747 g (2)/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:
A method for measuring the solubility of (2) in (1) was based on the use of tritium tracer to monitor the recovery of (2) in a conventional gravimetric method and to measure tritium distribution between the aqueous and the organic phases.

Source and Purity of Materials:
(1) Source not specified; thiophene free regent; recrystallized three times.
(2) HTO at 5 Ci/mL, New England Corp.; diluted to about 1 mCi/mL.

Estimated Error:
Solubility: better than 1% (type of error not specified).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. K. Rosenbaum and J. H. Walton, J. Am. Chem. Soc. **52**, 3568 (1930).

Variables:
Temperature: 10 °C–60 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g (1)
10	1.95	0.0451
20	2.48	0.0573
30	3.22	0.0746
40	4.12	0.0953
50	5.48	0.1271
60	7.05	0.1637

Auxiliary Information

Method/Apparatus/Procedure:
The organic phase was first saturated by shaking with water in a flask at a high temperature. The mixture was then allowing the flask to cool in a thermostat to the desired temperature, with the resulting separation of excess water. After 1 day or more the solution was allowed to react with added calcium hydride in dry solvent. Hydrogen was evolved and the gas volume was read.

Source and Purity of Materials:
(1) Source not specified; reagent grade; free from thiophene; boiling point 79.6 °C, melting point 5.4 °C; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. Sada, S. Kito, and Y. Ito, J. Chem. Eng. Data **20**, 373 (1975).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 2.0403 mL (1)/L (2).

Auxiliary Information

Method/Apparatus/Procedure:
Sudan IV was used to dye (1). The experimental apparatus and procedure used in this work was similar to those of Sobotka and Khan.[1] To make measurements more accurate, the apparatus used consisted of a 1-L dissolution flask and 2-mL microburet. The scale was calibrated in advance by use of mercury. The dissolution flask was immersed in a water bath controlled thermostatically at 25 °C. To avoid condensation of (1) from the gas phase in the dissolution flask was kept 1 °C higher than that of the liquid phase. The dissolution flask and the microburet were connected tightly.

Source and Purity of Materials:
(1) Source not specified; reagent grade; used as received; purity not specified.
(2) Pure.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: less than 0.008 mL (1)/L sln (type of error not specified).

References:
[1]H. Sobotka and J. Kahn, J. Am. Chem. Soc. **53**, 2935 (1948).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, S. Arakawa, M. Araki, and T. Deguchi, Bull. Chem. Soc. Jpn. **57**, 1539 (1984).

Variables:
One temperature: 25 °C

Prepared By:
G. T. Hefter

Experimental Values

The solubility of benzene in water at 25 °C was reported to be $2.07 \cdot 10^{-2}$ mol (1)/L sln.

Assuming a solution density of 1.00 kg/L this corresponds to a solubility of 0.162 g (1)/100 g sln, $x_1 = 3.73 \cdot 10^{-4}$, calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus used is described in detail in Sanemasa *et al.*[1] The method involves the introduction of solute vapor (1) into liquid (2) by bubbling air through liquid (1) using a recirculating pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analyzed by solvent extraction-UV spectrophotometry.

Source and Purity of Materials:
(1) Analytical reagent grade source and purity not stated, used without further purification.
(2) Deionized and redistilled; no further details given.

Estimated Error:
Not specified.

References:
[1]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 5 °C–45 °C

Prepared By:
G. T. Hefter

Experimental Values

Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)[a]	g (1)/100 g sln (compiler)[a]	$10^3 \cdot$ mol (1)/L sln
5	3.73	0.162	20.7
15	3.65	0.158	20.2 ± 0.3
25	3.74	0.162	20.7[b] ± 0.1
35	3.94	0.171	21.8 ± 0.6
45	4.15	0.180	22.8 ± 0.5

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).
[b]No error estimate given.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail and in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid components.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 99.5%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Variables:
Temperature: 15 °C–45 °C

Prepared By:
M. C. Haulait-Pirson and G. T. Hefter

Experimental Values
Solubility of benzene in water

t/°C	$10^4 \cdot x_1$[a]	g (1)/100 g sln[a]	g (1)/L
15	3.56	0.154	1.54 ± 0.04
25	3.72	0.161	1.61 ± 0.09
35	4.09	0.177	1.76 ± 0.06
45	4.32	0.187	1.85 ± 0.11

[a]Assuming the solution density to be that of pure water at the same temperature (Weast[1]).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel, respectively. The solute vapor, generated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/min. Solubility equilibria were attained within 5 min. Then portions of 10 mL of the aqueous solution were transferred into funnels to which 10 mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported. The solubility runs were made such that the temperature of the solute reservoir was made to vary while that of solvent phase was held constant. The solubility obeys Henry's law at constant solvent temperature. Solubility values were calculated from Henry's law constants.

Source and Purity of Materials:
(1) Analytical reagent grade used as purchased.
(2) Redistilled.

Estimated Error:
Given above.

References:
[1]*CRC Handbook of Chemistry and Physics*, 63rd, R. C. Weast, Editor (CRC Press, Boca Raton, Florida, 1982), p. pF-11.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values
Solubility of benzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$2.07 \cdot 10^{-2}$	0.1620	$3.74 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The apparatus used for preparing aqueous solutions saturated with hydrocarbon vapor was the same as that previously reported in Sanemasa *et al.*[1] The method was based on the introduction of phase (1) (by bubbling air through the mixture using circulating pump in a closed system) into 100 mL of water. After 10 min (at circulation rate of vapor of 1.5 L/min) equilibrium was attained, and a 30 mL portion of the saturated aqueous solution was transferred into three separatory funnels with 5 mL of benzene. Mixtures were analyzed by gas chromatography.

Source and Purity of Materials:
(1) Source not specified; analytical reagent grade; purity 99.5%; used as received.
(2) Deionized and redistilled.

Estimated Error:
Temperature: ±0.1 °C

References:
[1]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, K. Kitamura, and Y. Taniguchi, J. Phys. Chem. **93**, 4931 (1989).

Variables:
Temperature: 25.00 °C
Pressure: 0.1 MPa–400 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

t/°C	P/MPa	mol (1)/L sln	x_p/x_0 [a]	$10^3 \cdot g$ (1)/100 g sln (compilers)	$10^4 \cdot x_1$ (compilers)
25.00	0.1	$2.4 \cdot 10^{-2}$	1	1.87	4.33
	25		1.035	1.94	4.49
	50		1.054	1.98	4.57
	75		1.069	2.00	4.63
	100		1.073	2.01	4.65

[a] x_p/x_0 = relation of the solubility at high and normal pressure.

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water and a few drops of benzene were placed into a high pressure optical cell with a Teflon ball for stirring and described in Sawamura *et al.*[1] The sample was pressurized and shaken in a thermoregutated water bath for 5 h. The absorbance was measured with a Hitachi Model 340 double-beam spectrophotometer. Details of the apparatus, procedures, and purification were reported in Sawamura *et al.*[1] The solubility was calculated through the Lambert-Beer's law with use of the molar extinction coefficients. The ratios of the solubility at high and atmospheric pressures are the average of at least 3 measurements.

Source and Purity of Materials:
(1) Nacalai Tesque, Co.; shaken successively with H_2SO_4, Na_2CO_3 aq, H_2O, dried over $MgSO_4$, distilled.
(2) Not specified.

Estimated Error:
Temperature: ±0.01 °C.

References:
[1] S. Sawamura, K. Suzuki, and Y. Taniguchi, J. Sol. Chem. **16**, 649 (1987).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. H. Saylor, J. M. Stuckey, and P. M. Gross, J. Am. Chem. Soc. **60**, 373 (1938).

Variables:
Temperature: 30 °C and 35 °C

Prepared By:
A. Maczynski

Experimental Values

Solubility of benzene in water

t/°C	$10 \cdot {}^4x_1$ (compiler)	g (1)/100 g sln (compiler)	mol (1)/L sln
30	4.25	0.184	0.0236
35	4.38	0.190	0.0243

Auxiliary Information

Method/Apparatus/Procedure:
A large quantity of (1) was brought to equilibrium with a limited quantity of (2). Analysis were made by comparing the readings of the solutions in a Zeiss combination interferometer with those of known standards made by dissolved weighed quantities of (1) in known weights of (2) as described in Gross and Saylor.[1]

Source and Purity of Materials:
(1) Source not specified; purified; melting point 5.48 °C.
(2) Distilled.

Estimated Error:
Presumably:
Temperature: ±0.01 °C.
Solubility: ±0.005 g (1)/100 g (2).

References:
[1] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1747 (1931).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. Schatzberg, J. Phys. Chem. **67**, 776 (1963).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

The solubility of water in benzene at 20 °C was reported to be 532 mg (2)/kg (1).

The corresponding mass percent and mole fraction calculated by the compilers are 0.0532 g (2)/100 g sln and $2.30 \cdot 10^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a serum cap-sealed 4-oz. brown glass bottle immersed in a water bath, (1) was saturated with (2) at 20±0.02 °C for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe pushed about 2/3 of the way into the hydrocarbon liquid. Stabilized Karl Fischer reagent diluted to a titer of 1.0–1.3 mg (2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a dead-stop end-point using a Beckman KF3 automatic titrimeter with a 5-mL microburet.

Source and Purity of Materials:
(1) Matheson, Coleman and Bell Chromatoquality reagent 99 + mole %; used as received.
(2) Distilled and deionized.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: ±3 mg(2)/kg(1) (type of error not specified).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Variables:
One temperature: 23.5 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Values

Solubility of benzene in water

t/°C	g (1)/100 g sln	$10^4 \cdot x_1$ (compiler)
23.5	0.188±0.005*[a]	4.34
	0.188±0.009[b]	4.34
	0.182±0.007[c]	4.20
	0.193±0.011[d]	4.45

*Values determined for different masses of (1) coated into the inert support:
[a] — 0.014; [b] — 0.0154; [c] — 0.0124; [d] — 0.0464; [e] — 0.0526 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:
An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (Chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas supply). Water was forced through the column by the pressure of the column by the pressure of the compressed gas (~14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e., length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.

Source and Purity of Materials:
(1) Spectral grade used without further purification.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 4% (average standard deviation).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. P. Singh and R. Sah, Indian J. Chem. **16A**, 692 (1978).

Variables:
One temperature: 303.15 K

Prepared By:
A. Maczynski

Experimental Values

The solubility of water in benzene at 303.15 K was reported to be 0.064 g (2)/mol(1).

The corresponding mass percent and mole fraction, x_2, values calculated by compiler are 0.082 g (2)/100 g sln and 0.0035.

Auxiliary Information

Method/Apparatus/Procedure:
The titrations were carried out in well stoppered volumetric flasks in order to check for loss due to vaporization. Shaking after each addition of water was done in an ultrasonic shaker for at least 30 min. The contents were equilibrated in a thermostat. The final end point was determined when a second phase appeared and the volume of the water added was noted. Each titration was repeated at least three times to check the reproducibility of the results.

Source and Purity of Materials:
(1) BDH, analar quality; purified; purity not specified.
(2) Conductivity water.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: ±5% (type of error not specified).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
V. G. Skripka, Tr. Vses. Neftegazov. Nauch. Issled. Inst. **61**, 139 (1976).
R. G. Sultanov and V. G. Skripka, Zh. Fiz. Khim. **47**, 1035 (1973).

Variables:
Temperature: 225 °C–260 °C
Pressure: 4.7 MPa–78.5 MPA

Prepared By:
A. Maczynski

Experimental Values

Solubility of water in benzene

t/°C	x_2	g (2)/100 g sln (compiler)	P/kg·cm^{-2}	P/MPa (compiler)
225	0.256	7.35	48	4.7
225	0.250	7.14	100	9.8
225	0.242	6.86	150	14.7
225	0.228	6.37	200	19.6
225	0.227	6.34	300	29.4
225	0.217	6.01	400	39.2
225	0.209	5.74	500	49.0
225	0.200	5.45	600	58.8
225	0.191	5.16	700	68.6
225	0.183	4.91	800	78.5
250	0.410	13.81	75	7.4
250	0.399	13.27	100	9.8
250	0.378	12.29	150	14.7
250	0.361	11.52	200	19.6
250	0.332	10.28	300	29.4
250	0.314	9.55	400	39.2
250	0.312	9.47	500	49.0
250	0.291	8.64	600	58.8
250	0.280	8.23	700	68.6
250	0.270	7.86	800	78.5
260	0.491	18.19	84.5	8.3
260	0.479	17.49	100	9.8
260	0.442	15.44	150	14.7
260	0.416	14.10	200	19.6
260	0.381	12.43	300	29.4
260	0.363	11.61	400	39.2
260	0.352	11.13	500	49.0
260	0.342	10.70	600	58.8
260	0.332	10.28	700	68.6
260	0.321	9.83	800	78.5

Auxiliary Information

Method/Apparatus/Procedure:
The experimental technique was described in Sultanov *et al.*[1] No details reported in the paper.

Source and Purity of Materials:
(1) Source not specified, chemical reagent grade; purity not specified; used as received.
(2) Distilled.

Estimated Error:
Not specified.

References:
[1]R. G. Sultanov, V. G. Skripka, and A. Yu. Namiot, Gazov. Prom. **4**, 6 (1971).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. A. K. Staveley, J. H. E. Jeffes, and J. A. E. Moy, Trans. Faraday Soc. **39**, 5 (1943).

Variables:
Temperature: 24 °C–71 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values
Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/kg(1)	g (2)/100 g sln (compiler)
24.7	2.96	0.685	0.0685
41.4	5.23	1.213	0.1212
44.0	5.88	1.296	0.1294
50.4	6.97	1.619	0.1616
58.2	8.91	2.073	0.2069
58.5	9.41	2.190	0.2185
71.0	12.74	2.976	0.2967

Auxiliary Information

Method/Apparatus/Procedure:
About 50 mL of (1) was introduced into a clean dry glass tube about 3.5 cm in diameter with a narrow inlet, a small amount of (2) was added from a weighted pipette, and the tube at once sealed off. It was then agitated at a sufficiently high temperature until all (2) had gone into solution, placed in a bath of water, and allowed to cool slowly. The temperature at which (1) was saturated with respect to (2) was taken to be that at which opalescence appeared.

Source and Purity of Materials:
(1) Source not specified; dried over sodium wire; distilled from sodium powder.
(2) Not specified.

Estimated Error:
Temperature: ±1.5 °C.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. A. K. Staveley, R. G. S. Johns, and B. C. Moore, J. Chem. Soc. 2516 (1951).

Variables:
Temperature: 22.7 °C–73.2 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$	G(2)/100 g sln (compiler)
22.7	2.606	0.0602
30.5	3.674	0.0849
33.0	3.784	0.0875
40.6	5.041	0.1167
41.9	5.153	0.1193
45.9	6.064	0.1405
51.9	6.902	0.1600
52.2	7.078	0.1641
53.2	7.211	0.1672
54.7	7.521	0.1744
60.9	9.294	0.2158
65.3	10.50	0.2441
67.2	11.21	0.2607
73.2	13.02	0.3032

The smoothing equation of the authors is:

$$\log x_2 = 2.237 - 1427/(t/°C + 273.1)$$

Auxiliary Information

Method/Apparatus/Procedure:
A synthetic mixture of known amounts of (2) and (1) was heated in a sealed tube until homogeneous and then the temperature of the phase splitting on cooling was determined. The apparatus and procedure are described in Stavely *et al.*[1]

Source and Purity of Materials:
(1) Source not specified; stored over phosphoric oxide.
(2) Not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±0.2% (type of error not specified).

References:
[1]Stavely, Jeffes, and Moy, Trans. Faraday Soc. **39**, 5 (1943).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. S. Stearns, H. Oppenheimer, E. Simon, and W. D. Harkins, J. Chem. Phys. **15**, 496 (1947).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and D. Shaw

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 0.086 and 0.085 g (1)/100 g sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.085 g (1)/100 g sln and $2.0 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
Mixtures of (1) in (2) of known composition were shaken for at least 48 h. The turbidity was then measured with a photometer. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.

Source and Purity of Materials:
(1) Not specified. (2) Not specified.

Estimated Error:
Temperature: ±3 °C.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. M. Stephenson, J. Chem. Eng. Data **37**, 80 (1992).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of benzene in water

t/°C	g (1)/100 g sln	$10^3 \cdot x_1$ (compilers)
25.0	0.157	0.363
	0.158	0.365
	0.193	1.93
	0.2	2.0

Solubility of water in benzene

t/°C	g (2)/100 g sln	$10^3 \cdot x_2$ (compilers)
25.0	0.067	2.9
	0.076	3.3
	0.09	3.9
	0.2	8.6

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Benzene (1) and water (2) were brought into equilibrium at a given temperature in a thermostat, and samples of each layer were removed by a syringe for analysis. To each sample a higher boiling organic compound was added as a standard and the ratio of peaks was measured by gas chromatography.[1,2] Temperature was measured by a calibrated thermometer accurate to 0.1 °C The results reported above are the part of various ternary solubility measurements.

Source and Purity of Materials:
(1) Aldrich Chemical Co.; purity>99.9 mass%.
(2) Not stated.

Estimated Error:
Temperature: ±0.1 °C.

References:
[1]R. M. Stephenson, J. Stuart, and M. Tabak, J. Chem. Eng. Data **29**, 287 (1984).
[2]R. M. Stephenson and J. Stuart, J. Chem. Eng. Data **31**, 56 (1986).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. A. Taha, R. D. Grigsby, J. R. Johnson, S. D. Christian, and H. E. Affsprung, J. Chem. Educ., **43**, 432 (1966).

Variables:
One temperature: 25 °C

Prepared By:
G. T. Hefter

Experimental Values

The solubility of benzene in water at 25 °C was reported as 0.022 mol/L sln.

The corresponding mass percent and mole fraction solubility, x_1, calculated by the compiler are, assuming a solution density of 1.00 kg/L, 0.16 g (1)/100 g sln and $4.0 \cdot 10^{-4}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:
Solubility of (1) in (2) was determined from vapor pressure measurements. 190 mL of pure water were placed in a glass manometric apparatus of known vapor volume. The apparatus is described in detail in the paper. The apparatus was evacuated, benzene added (probably as a liquid), and the pressure measured.

Source and Purity of Materials:
(1) Source and purity not specified.
(2) Pure; purity not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. N. Tarassenkow and E. N. Poloshinzewa, Ber. Dtsch. Chem. Ges., **65**, 184 (1932).

Variables:
Temperature: 5 °C–73 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
5	1.0	0.024
9.5	1.5	0.034
14.5	1.8	0.041
22.5	2.6	0.060
32	3.5	0.082
40	4.4	0.102
56	7.8	0.181
67.5	10.8	0.251
73	12.9	0.300

Auxiliary Information

Method/Apparatus/Procedure:
The method of Alexjew[1] method was used. No additional details were reported in the paper.

Source and Purity of Materials:
(1) Kahlbaum, CP; dried over calcium chloride and distilled from sodium, purity not specified.
(2) Not specified.

Estimated Error:
Solubility: ±0.01% (not specified).

References:
[1]W. Alexejew, Wied. Ann. Physik **28**, 35 (1886).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. H. Thompson and J. R. Snyder, J. Chem. Eng. Data, **9**, 516 (1964).

Variables:
Temperature: 37.9 °C–204.3 °C
Pressure: 7 MPa and 34.6 MPa

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Values

Mutual solubility of benzene and water at 1000 psig (7 MPa compiler)

t/°F	t/°C (compiler)	$10^4 \cdot x_1$	$10^4 \cdot x_2$	g (1)/100 g sln (compiler)	g (2)/100 g sln (compiler)
99.9	37.7	4.33	41.6	0.187	0.0962
99.9	37.7	4.61	41.8	0.200	0.0967
100.1	37.8	4.54	46.6	0.197	0.1078
100.3	37.9	4.34	48.7	0.188	0.1127
101.0	38.3	4.60	42.1	0.199	0.0974
101.5	38.6	—	43.3	—	0.1002
160.3	71.2	6.63	124	0.287	0.289
218.0	103.3	9.84	—	0.425	—
219.0	103.8	8.56	274	0.370	0.645
280.0	137.8	—	558	—	1.344
280.3	137.9	14.3	—	0.617	—
281.0	138.3	18.6	—	0.802	—
339.3	170.7	41.6[a]	—	1.780	—
339.3	170.7	42.7[a]	—	1.826	—
340.0	171.1	44.2[a]	1000	1.889	2.498
340.3	171.3	46.5[a]	—	1.986	—
341.0	171.7	36.0[a]	—	1.543	—
396.3	202.4	85.3	—	3.60	—
397.3	202.9	—	1770	—	4.724
398.0	203.3	94.2[a]	—	3.96	—
399.0	203.9	72.6	—	3.07	—
399.7	204.3	81.0	—	3.42	—

[a]Results known to be high due to a high analytical blank.

Mutual solubility of benzene and water at 500 psig (34.6 MPa compiler)

t/°F	t/°C (compiler)	$10^4 \cdot x_1$	$10^4 \cdot x_2$	g (1)/100 g sln (compiler)	g (2)/100 g sln compiler)
100.3	37.9	5.61	38.1	0.243	0.0881
159.7	70.9	8.95	—	0.387	—
160.3	71.3	—	110	—	0.256
161.0	71.7	—	105	—	0.244
219.7	104.3	14.1	—	0.609	—
220.7	104.8	—	263	—	0.619
279.3	137.4	22.8	505	0.981	1.211
339.3	170.7	43.1	959	1.843	2.387
400.7	204.8	98.3	1530	4.13	3.998
459.7	237.6	248	4320	9.93	14.92
460.7	238.1	265	4600	10.56	16.42

Author's smoothed values of the mutual solubility of benzene and water at 1000 psig (7 MPa)

t/°F	t/°C (compiler)	$10^4 \cdot x_1$	$10^4 \cdot x_2$	g (1)/100 g sln (compiler)	g (2)/100 g sln (compiler)
100	38	4.46	42.3	0.193	0.0978
160	71	6.65	121	0.288	0.282
220	104	10.1	274	0.436	0.645
280	138	18.6	558	0.801	1.34
340	171	36.0	1000	1.54	2.50
400	204	82.0	1780	3.46	4.75

Author's smoothed values of the mutual solubility of benzene and water at 5000 psig (34.6 MPa)

t/°F	t/°C (compiler)	$10^4 \cdot x_1$	$10^4 \cdot x_2$	g (1)/100 g sln (compiler)	g (2)/100 g sln compiler)
100	38	5.61	38.1	0.243	0.0880
160	71	9.05	106	0.392	0.246
220	104	14.1	245	0.608	0.575
280	138	22.8	500	0.980	1.20
340	171	43.0	905	1.84	2.24
400	204	98.0	1620	4.11	4.45
460	238	255	4500	10.20	15.90

Auxiliary Information

Method/Apparatus/Procedure:

About 70 mL each of (1) and (2) were placed in a high-pressure equilibrium cell. The cell was installed in the phase-contacting equipment, pressurized with nitrogen, heated and kept horizontal with no agitation for at least 24 h, then rotated and kept vertical for 3 h to ensure complete phase separation. Each phase was sampled (20 mL) and the sample volume measured under the experimental conditions. The (1)-rich phase was analyzed for (2) by the Karl Fischer method and the (2)-rich phase for (1) via combustion at 1450 °F–1500 °F over CuO, absorption of CO_2 and back-titration of NaOH.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; pure grade, 99+ mole%; used as received.
(2) Distilled and redistilled in the absence of carbon dioxide.

Estimated Error:

Not specified.

Components:

(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. Tsonopoulos and G. M. Wilson, AIChE J., **29**, 990 (1983).

Variables:

Temperature: 313–473 °C
Pressure: 0.03–3.0 MPa

Prepared By:

G. T. Hefter

Experimental Values

Solubility of benzene in water

T/K	$10^3 \cdot x_1$	g (1)/100 g sln (compiler)	P^a/MPa
313.15	0.4435	0.192	0.03054
373.15	0.949	0.412	0.2758
423.15	2.42	1.05	1.0549
473.15	5.40	2.34	3.020

Solubility of water in benzene

T/K	$10^2 \cdot x_2$	g (2)/100 g sln (compiler)	P^a/MPa
313.15	0.471, 0.501	0.112[b]	0.03054
373.15	1.81, 2.08	0.448[b]	0.2758
423.15	7.13	1.64	1.0549
473.15	18.5	4.26	3.020

[a]Absolute pressure.
[b]Average value.

The three phase critical point was reported: 541.7 K, 9.42 MPa, $x_1 = 2.528 \cdot 10^{-2}$ [10.1 g (1)/100 g sln, compiler].

The authors are also report equations fitted to their own and literature data over the range 273 K–542 K, viz.

$$\ln x_1 = -170.04018 + 6922.912/T + 24.398795 \cdot \ln T$$

$$\ln x_2 = -1.64055 = 2029.41/T + 0.00900544 \cdot T$$

Auxiliary Information

Method/Apparatus/Procedure:

All experimental details are given in an Appendix deposited in a Documentation Center rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, while that of (2) in (1) was measured by the Karl Fischer titration.

Source and Purity of Materials:

(1) No details given.
(2) No details given.

Estimated Error:

Temperature: not stated.
Solubility: ±5% relative; repeatability of replicable analyses.
Pressure: ±1%; type or error not stated.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O [7732-18-5]

Original Measurements:
V. V. Udovenko and L. P. Aleksandrova, Zh. Fiz. Khim., **37**, 52 (1963).

Variables:
Temperature: 20 °C–79.5 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln
20.0	4.85	0.210
30.0	5.24	0.227
40.5	5.73	0.248
44.5	5.98	0.259
56.5	6.65	0.288
60.0	6.93	0.300
65.0	7.37	0.319
79.5	8.62	0.373

Auxiliary Information

Method/Apparatus/Procedure:
The polythermic method of Alekseev was used. No details were reported in the paper.

Source and Purity of Materials:
(1) Source not specified; dried over metallic sodium, and distilled; n_D^{20} 1.5013; d_4^{30} 0.8661.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. P. Uspenskii, Neft. Khoz., **11-12**, 713 (1929).

Variables:
Temperature: 10 °C and 22 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

Solubility of benzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	g (1)/100 g sln
10	4.04	0.175 ± 0.001
22	4.306	0.1865 ± 0.0015

Solubility of water in benzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln
10	2.2	0.051 ± 0.0011
22	2.86	0.0662 ± 0.0008

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by titration. The solubility of (2) in (1) was determined by the method of Clifford.[1] Dried air was passed through the vessel with a saturated solution of (2) in (1) and U-tubes with $CaCl_2$ and next the absorbed (2) was weighed.

Source and Purity of Materials:
(1) Source not specified; boiling point 79.8 °C at 740 mm Hg,; d_4^{30} 0.8768; d_4^{10} 0.8887.
(2) Not specified.

Estimated Error:
Solubility: see experimental values above.

References:
[1]C. W. Clifford, Ind. Eng. Chem. **13**, 628 (1921).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Values

Solubility of ethylcyclohexane in water

T/K	mol (1)/g (2)	g (1)/100 g sln (compilers)	x_1 (compilers)
298.15	$(2.44 \pm 0.01) \cdot 10^{-5}$	0.1905	$4.40 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The equilibration was carried out in a modified vessel,[1] equipped with a magnetic stirrer. The temperature of the water bath as maintained constant within ±0.05 K. Equilibrium was obtained after 48 h and then the samples were analyzed by spectrophotometry.

Source and Purity of Materials:
(1) Commercial analytical grade reagent; purity >99% by glc; distilled through a column.
(2) Distilled water passed through an Amberlite CG 120+CG 400 ion-exchange column.

Estimated Error:
Temperature: ±0.05 K.
Solubility: as above.

References:
[1]F. Franks, M. Gent, and H. H. Johnson, J. Chem. Soc. 2716 (1963).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Wing and W. H. Johnston, J. Am. Chem. Soc., **79**, 864 (1957).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Values

The solubility of water in benzene at 25 °C was reported to be 0.0554 mL (2)/100 mL sln and 0.0635 mL (2)/100 g (1).

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.114 g (2)/100 g sln and $4.9 \cdot 10^{-3}$. The assumption that 1 mL sln= 874 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
A small amount of (2) was equilibrated with 20 mL of (1) using a Teflon stirrer in a 100 mL flask in a Sargent constant temperature bath. At the end of 2 h, the mixture was poured into a test tube immersed in the bath and the organic phase separated from water by gravity. The determination of THO in the organic phase was done by isotopic dilution with a large excess of H_2O. The tritium activities in the tritiated water samples were determined by the acetylene method described in Wing and Johnson.[1]

Source and Purity of Materials:
(1) Source not specified, chemical grade; redistilled in a column of 50 theoretical plates; purity not specified.
(2) Tracerlab, Inc., tritiated water with an activity of approximately 1 μCi/mL.

Estimated Error:
Temperature: ±0.02 °C.
Solubility: 0.9% (standard deviation from 6 determinations).

References:
[1]J. Wing and W. H. Johnson, Science **121**, 674 (1955).

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. D. Worley, Can. J. Chem., **45**, 2465 (1967).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Values

The solubility of benzene in water at 25 °C was reported to be 2.17 g (1)/L sln.

The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 0.217 g (1)/100 g sln and $5.01 \cdot 10^{-4}$. The compiler's calculation assumes a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:
The isotopic solute transfer technique of Christian *et al.*[1,2] was used.

This method consists of vapor phase equilibration of water with solutions of benzene-dinonylphthalate in closed containers. The benzene absorbance was measured at 254 nm with a Cary 14 spectrophotometer.

Source and Purity of Materials:
(1) Source not specified; reagent grade; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±0.2 °C.

References:
[1]S. D. Christian *et al.*, J. Chem. Educ. **40**, 419 (1963).
[2]S. D. Christian, H. E. Affsprung, and J. R. Johnson, J. Chem. Soc. 1896 (1963).

3.2. Benzene with Heavy Water

Components:
Benzene; C_6H_6; [71-43-2]
(2) Heavy water (deuterium oxide); D_2O; [7789-20-0]

Original Measurements:
P. Backs and S. Goldman, J. Phys. Chem. **85**, 2975 (1981).

Variables:
Temperature: 283 K–313 K

Prepared By:
A. Maczynski

Experimental Values

Solubility of heavy water in benzene

T/K	$10^3 \cdot x_2$	Std. dev	$10^3 \cdot g$ (2)/100 g sln (compiler)
283	1.70	0.03	0.4364
288	1.91	0.03	0.490
293	2.17	0.04	0.557
298	2.68	0.06	0.689
303	3.02	0.04	0.776
308	3.56	0.04	0.915
313	4.12	0.08	1.0574

Auxiliary Information

Method/Apparatus/Procedure:
In a 175-mL milk-dilution bottle fitted with a Bakelite screw cap and a Teflon insert and rotated end-over-end, (1) was equilibrated with an excess of (2), sampled with Hamilton syringes and titrated in an Aquatest II automatic Karl Fischer Titrator.

Source and Purity of Materials:
(1) Certified grade; washed successively with concentration $H_2SO_4H_2O$, 1 N NaOH, again H_2O, dried with silica gel, and distilled; d^{25} 0.87365.
(2) Obtained from the manufacturer; minimum isotopic purity of 99.7 at. % D.

Estimated Error:
Temperature: ±0.01 K.
Solubility: standard deviation calculated from 25–36 determinations reported above.

Components:
(1) Benzene; C_6H_6; [71-43-2]
(2) Heavy water (deuterium oxide); D_2O; [7789-20-0]

Original Measurements:
K. Bröllos, K. Peter, and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **74**, 682 (1970).

Variables:
Pressure and temperature on one phase-two phase boundary

Prepared By:
C. L. Young

Experimental Values

Values of pressure and temperature on the one phase-two phase boundary

T/K	P/bar	g (1)/100 g sln (compiler)	x_1
339.10	2445	0.250	56.5
337.50	2300		
333.40	2000		
328.00	1750		
323.90	1530		
314.90	1100		
308.40	840		
303.80	655		
300.10	490		
295.60	220		
326.10	170		
315.90	158		
355.20	2855	0.546	82.4
351.00	2600		
348.20	2450		
342.40	2095		
337.90	1850		
332.40	1585		
330.40	1480		
324.90	1300		
319.60	1100		
311.80	790		
303.40	521		
297.00	300		
296.20	250		
300.20	181		
312.20	166		
325.20	182		
330.30	2750	0.755	92.3
327.40	2600		
322.90	2300		
318.90	2000		
310.00	1500		
313.10	1700		
304.40	1200		
298.90	990		
296.40	840		
288.10	540		
281.00	290		
275.40	168		

Auxiliary Information

Method/Apparatus/Procedure:
Measurements were made in a steel optical cell within an aluminum block furnace. The cell contents were stirred magnetically. Pressure was measured using a movable piston and Bourdon gauge. Temperature was measured with a steel-sheathed thermocouple. Components were charged into the cell and the transition from one phase to two phases was observed visually.

Source and Purity of Materials:
(1) Merck sample purity 99.9 mole %.
(2) Isostopic purity 99.7 mole %.

Estimated Error:
Temperature: $\Delta T/\mathrm{K} = \pm 0.1$.
Pressure: $\Delta P/P = \pm 0.01$ (estimated by compiler).

4. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

Benzene + water E485, 494-549
Benzene + heavy water 549-550

5. Registry Number Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

[71-43-2]	C_6H_6	Benzene	E485-E493, 494-550
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[7789-20-0]	D_2O	Heavy water (deuterium oxide)	549-550

6. Author Index

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