IUPAC-NIST Solubility Data Series 69. Ternary Alcohol–Hydrocarbon–Water Systems

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The mutual solubilities of ternary systems containing alcohols, hydrocarbons and water are reviewed. An exhaustive search of the literature was attempted for numerical data on all alcohols and hydrocarbons which are liquid at STP. Data were found for alcohols with up to nine carbon atoms, but mostly with fewer than four carbons. Data for a variety of hydrocarbon structural types were found including alkane, alkene, and arene. A total of 205 original studies treating 116 ternary systems which have been published through 1992 are compiled. For 47 systems sufficient data were available to allow critical evaluation. All solubility data are expressed as mass and mole fractions as well as the originally reported units. Similar reviews of the related binary systems have previously been prepared for the Solubility Data Series. © *1999 American Institute of Physics and American Chemical Society.* [S0047-2689(99)00304-9]

Key words: aqueous solutions; hydrocarbons; solubility alcohols.

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1. Preface to the Volume

This volume of IUPAC Solubility Data Series on ternary alcohol–hydrocarbon–water systems is the continuation of previous works on binary systems. Alcohol–water systems were presented as Vol. 15 of the Series, Ref. 1; hydrocarbon–water systems were presented as Vols. 37 and 38 of the Series, Refs. 2 and 3 and alcohol–hydrocarbon systems were presented as Vol. 56 of the Series, Ref. 4.

This volume surveys solubility data (along saturation curve and phases in equilibrium) which have been published in the open literature up to the end of 1992. The alcohols are those to nine carbon atoms, the most common are methanol, ethanol, propanols, and butanols. The hydrocarbons include those with three or more carbon atoms and of all structural types (aliphatic, aromatic, unsaturated, etc.) which are liquids at room temperature and pressure.

A total of 205 original studies of 116 ternary systems are compiled. Components of these systems were always well-defined substances. From these, it has been possible to make critical evaluations for 47 systems. Only numerical data are given because data published originally in graphical form are inherently imprecise, especially given the high precision of the tabulated data for many systems. The literature contains a large amount of imprecise and conflicting data. Where possible, recommended or tentative values of composition along saturation curves and for phases in equilibrium are given, but and in many cases this cannot be done because of insufficient information. This volume is the result of a careful search of the chemical literature. The goal of that search was to include all published data for the systems indicated in the title. Each Critical Evaluation includes a closing date for the literature for that system, generally December, 1992. In spite of these efforts, some published measurements may have been missed. The editors will appreciate having their attention brought to any omitted source of solubility data for inclusion in future volumes.

For purposes of comparison, all original results are expressed in mass and mole fraction as well as in the units given by the original investigators. Conversions, where they have been made, are clearly attributed to the compiler and the sources of any data not provided by the original investigators are specified. Definitions of mass and mole fraction as well as their relation to other common measures of solubility are given in the Introduction to the Solubility Data Series: Solubility of Liquids in Liquids in this volume. A table of conversion formulas is included at the end of the Introduction.

The reported ternary data often form miscibility gaps with one pair of partially miscible components (type 1) e.g., ethanol–hydrocarbon–water or propanol–hydrocarbon–water systems or miscibility gap with two pairs of partially miscible components (type 2) e.g., methanol–hydrocarbon–water or 1-butanol–hydrocarbon–water systems. In this volume the alcohol is reported always as the first component, the hydrocarbon as the second, and water as the third. For each group (alcohols, hydrocarbons), substances are ordered by increasing number of carbon atoms. In brackets, after each compound name synonyms are given. Each system begins on a separate page; first, the critical evaluation is presented together with a graphical representation of the system at one selected temperature. This is followed by compilation of original papers. Critical evaluations are presented only for systems where two or more independent determinations of solubility allow comparison of experimental data. The concentration along the saturation curve as well as the concentration of phases in equilibrium are always expressed in mole and mass fractions of alcohol and hydrocarbon. Concentration of water may be calculated from the mass balance (sum of concentration is always equal 1.0). The indexes $'$ and $''$ express the phase number; $'$ describes organic-rich or hydrocarbon-rich phase, while $''$ describes water-rich or hydrocarbon-poor phase. Among the references in several evaluations occurs the Russian compilation of Kafarov (ed.), ''Spravochnik po Rastvorimosti,''[5] which contains only numerical data without any explanatory text; the English translation of this compilation was published as a handbook on solubility.[6]

The editors would like to thank Andrzej Bok (Thermodynamics Data Center, Warsaw, Poland) for preparing computer programs for presentation of the tables; Professor John W. Lorimer (Ontario, Canada) for valuable discussions and for preparing the addresses of translated Russian papers and all members of IUPAC Commission on Solubility Data (Vol. 8) for discussions.

1.1. References to the Preface

[1] A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

[2] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

[4] D. G. Shaw, A. Skrzecz, J. W. Lorimer, and A. Maczynski, eds., *Solubility Data Series*, Vol. 56, Alcohols with Hydrocarbons (Pergamon, New York, 1994).

[5] V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskva, 1963).

[6] H. Stephen and T. Stephen, eds., *Solubilities of Inorganic and Organic Compounds* (Pergamon, New York, 1963).

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

2.1. The Nature of the Project

The Solubility Data project (SDP) has as its aim a comprehensive review of published data for solubilities of gases, liquids, and solids in liquids or solids. Data of suitable precision are compiled for each publication on data sheets in a uniform format. The data for each system are evaluated and, where data from independent 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

The formats for the compilations and critical evaluations have been standardized for all volumes. A description of these formats follows.

2.2.1. Compilations

The format used for the compilations is, for the most part, self-explanatory. A compilation sheet is divided into boxes, with detailed contents described below.

Components

Each component is listed according to IUPAC name, formula, and Chemical Abstracts (CA) Registry Number. The Chemical Abstracts name is also included if this differs from the IUPAC name, as are trivial names if appropriate. IUPAC and common names are cross-referenced to Chemical Abstracts names in the System Index.

The formula is given either in terms of the IUPAC or Hill[1] system and the choice of formula is governed by what is usual for most current users: i.e., IUPAC for inorganic compounds, and Hill system for organic compounds. Components are ordered on a given compilation sheet according to:

(a) saturating components;
(b) nonsaturating components in alphanumerical order;
(c) solvents in alphanumerical order.

The saturating components are arranged in order according to the IUPAC 18-column periodic table with two additional rows:

Columns 1 and 2: H, alkali elements, ammonium, alkaline earth elements

Columns 3 to 12: transition elements

Columns 13 to 17: boron, carbon, nitrogen groups; chalcogenides, halogens

Column 18: noble gases

Row 1: Ce to Lu

Row 2: Th to the end of the known elements, in order of atomic number.

Organic compounds within each Hill formula are ordered in the following succession:

(a) by degree of unsaturation
(b) by order of increasing chain length in the parent hydrocarbon
(c) by order of increasing chain length of hydrocarbon branches
(d) numerically by position of unsaturation
(e) numerically by position by substitution
(f) alphabetically by IUPAC name.

Example:

C_5H_8	cyclopentane
	2-methyl-1,3-butadiene
	1,4-pentadiene
	1-pentyne
C_5H_{10}	cyclopentane
	3-methyl-l-butene
	2-methyl-2-butene

	1-pentene
	2-pentene
C_5H_{12}	2,2-dimethylpropane
	2-methylbutane
	pentane
$C_5H_{12}O$	2,2-dimethyl-l-propanol
	2-methyl-l-butanol
	2-methyl-2-butanol
	3-methyl-l-butanol
	3-methyl-2-butanol
	1-pentanol
	2-pentanol
	3-pentanol
$C_6H_{12}O$	cyclohexanol
	4-methyl-l-penten-3-ol
	1-hexen-3-ol
	4-hexen-3-ol

Deuterated (^{2}H) compounds follow immediately the corresponding H compounds.

Original Measurements

References are abbreviated in the forms given by Chemical Abstracts Service Source Index (CASSI). Names originally in other than Roman alphabets are given as transliterated by Chemical Abstracts. In the case of multiple entries (for example, translations) an asterisk indicated the publication used for compilation of the data.

Variables

Ranges of temperature, pressure, etc., are indicated here.

Prepared by

The names of all compilers are given here.

Experimental Data

Components are described as (1), (2), etc., as defined in the ‘‘Components’’ box. Data are reported in the units used in the original publication, with the exception that modern names for units and quantities are used; e.g., mass percent for weight percent; mol dm^{-3} for molar; etc. In most cases, both mass and molar values are given. Usually, only one type of value (e.g., mass percent) is found in the original paper, and the compiler has added the other type of value (e.g., mole percent) from computer calculations based on 1989 atomic weights.[2] Temperatures are expressed as t/°C, t/°F, or T/K as in the original; if necessary, conversions to T/K are made, sometimes in the compilations, and always in the critical evaluation. However, the author’s units are expressed according to IUPAC recommendations[3] as far as possible.

Errors in calculations, fitting equations, etc., are noted, and where possible corrected. Material inserted by the compiler is identified by the word ‘‘compiler’’ or by the compiler’s name in parentheses or in a footnote. In addition, compiler-calculated values of mole or mass fractions are included if the original data do not use these units. If densities are reported in the original paper, conversions from concentrations to mole fractions are included, but otherwise this is done in the evaluation, with the values and sources of the densities being quoted and referenced.

Details of smoothing equations (with limits) are included if they are present in the original publication and if the temperature or pressure ranges are wide enough to justify this procedure and if the compiler finds that the equations are consistent with the data.

The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure. In some cases graphs have been included, either to illustrate presented data more clearly, or if this is the only information in the original. Full grids are not usually inserted as it is not intended that users should read data from the graphs.

Method

The apparatus and procedure are mentioned briefly. Abbreviations used in Chemical Abstracts are often used here to save space, reference being made to sources of further detail if these are cited in the original paper.

Source and Purity of Materials

For each component, referred to as (1), (2), etc., the following information (in this order and in abbreviated form) is provided if available in the original paper: source and specified method of preparation; properties; degree of purity.

Estimated Error

If estimated errors were omitted by the original authors, and if relevant information is available, the compilers have attempted to estimate errors (identified by ‘‘compiler’’ or the compiler’s name in parentheses or in a footnote) from the internal consistency of data and type of apparatus used. Methods used by the compilers for estimating and reporting errors are based on Ku and Eisenhart.[4]

Comments and/or Additional Data

Many compilations include this section which provides short comments relevant to the general nature of the work or additional experimental and thermodynamic data which are judged by the compiler to be of value to the reader.

References

The format for these follows the format for the Original Measurements box, except that final page numbers are omitted. References (usually cited in the original paper) are given where relevant to interpretation of the compiled data, or where cross-reference can be made to other compilations.

2.2.2. Evaluations

The evaluator's task is to assess the reliability and quality of the data, to estimate errors where necessary, and to recommend ''best'' values. The evaluation takes the form of a summary in which all the data supplied by the compiler have been critically reviewed. There are only three boxes on a typical evaluation sheet, and these are described below.

Components

The format is the same as on the Compilation sheets.

Evaluator

The name and affiliation of the evaluator(s) and date up to which the literature was checked.

Critical Evaluation

(a) Critical text. The evaluator checks that the compiled data are correct, assesses their reliability and quality, estimates errors where necessary, and recommends numerical values based on all the published data (including theses, reports, and patents) for each given system. Thus, the evaluator reviews the merits or shortcomings of the various data. Only published data are considered. Documented rejection of some published data may occur at this stage, and the corresponding compilations may be removed.

The solubility of comparatively few systems is known with sufficient accuracy to enable a set of recommended values to be presented. Although many systems have been studied by at least two workers, the range of temperatures is often sufficiently different to make meaningful comparison impossible.

Occasionally, it is not clear why two groups of workers obtained very different but internally consistent sets of results at the same temperature, although both sets of results were obtained by reliable methods. In such cases, a definitive assessment may not be possible. In some cases, two or more sets of data have been classified as tentative even though the sets are mutually inconsistent.

(b) Fitting equations. If the use of a smoothing equation is justifiable the evaluator may provide an equation representing the solubility as a function of the variables reported on all the compilation sheets, stating the limits within which it should be used.

(c) Graphical summary. In addition to (b) above, graphical summaries are often given.

(d) Recommended values. Data are recommended if the results of at least two independent groups are available and they are in good agreement, and if the evaluator has no doubt as to the adequacy and reliability of the applied experimental and computational procedures. Data are reported as tentative if only one set of measurements is available, or if the evaluator considers some aspect of the computational or experimental method as mildly undesirable but estimates that it should cause only minor errors. Data are considered as doubtful if the evaluator considers some aspect of the computational or experimental method as undesirable but still considers the data to have some value where the order of magnitude of the solubility is needed. Data determined by an inadequate method or under ill-defined conditions are rejected. However, references to these data are included in the evaluation together with a comment by the evaluator as to the reason for their rejection.

(e) References. All pertinent references are given here, including all those publications appearing in the accompanying compilation sheets and those which, by virtue of their poor precision, have been rejected and not compiled.

(f) Units. While the original data may be reported in the units used by the investigators, the final recommended values are reported in SI units[3] when the data can be converted accurately.

2.3. Quantities and Units Used in Compilation and Evaluation of Solubility Data

2.3.1. Mixtures, Solutions and Solubilities

A *mixture*[5,6] describes a gaseous, liquid or solid phase containing more than one substance, where the substances are all treated in the same way.

A *solution*[5,6] describes a liquid or solid phase containing more than one substance, when for convenience one of the substances, which is called the *solvent*, and may itself be a mixture, is treated differently than the other substances, which are called *solutes*. If the sum of the mole fraction of the solutes is small compared to unity, the solution is called a *dilute solution*.

The *solubility* of a solute 1 (solid, liquid or gas) is the analytical composition of a saturated solution, expressed in terms of the proportion of the designated solute in a designated solvent.[7]

''Saturated'' implies equilibrium with respect to the processes of dissolution and demixing; the equilibrium may be stable or metastable. The solubility of a substance in metastable equilibrium is usually greater than that of the same substance in stable equilibrium. (Strictly speaking, it is the activity of the substance in metastable equilibrium that is greater.) Care must be taken to distinguish true metastability form supersaturation, where equilibrium does not exist.

Either point of view, mixture or solution, may be taken in describing solubility. The two points of view find their expression in the reference states used for definition of activities, activity coefficients and osmotic coefficients. Note that the composition of a saturated mixture (or solution) can be described in terms of any suitable set of thermodynamic components.

2.3.2. Physicochemical Quantities and Units

Solubilities of solids have been the subject of research for a long time, and have been expressed in a great many ways, as described below. In each case, specification of the temperature and either partial or total pressure of the saturating gaseous component is necessary. The nomenclature and units

TABLE 1. Interconversions between quantities used as measures of solubilities c-component systems containing c-1 solutes i and single solvent c (ρ—density of solution; M_i—molar masses of i. For relations for two-component systems, set summations to 0.)

	x_i	w_i	m_i	c_i
$x_i=$	x_i	$\dfrac{1}{1+\dfrac{M_i}{M_c}\left\{\dfrac{1}{w_i}-1+\sum_{j\neq 1}^{c-1}\left(\dfrac{M_c}{M_j}-1\right)\dfrac{w_j}{w_i}\right\}}$	$\dfrac{1}{1+\dfrac{1}{m_iM_c}+\sum_{j\neq i}^{c-1}\dfrac{m_j}{m_i}}$	$\dfrac{1}{1+\dfrac{1}{M_c}\left(\dfrac{\rho}{c_i}-M_i\right)+\sum_{j\neq i}^{c-1}\dfrac{c_j}{c_i}\left(1-\dfrac{M_j}{M_c}\right)}$
$w_i=$	$\dfrac{1}{1+\dfrac{M_c}{M_i}\left\{\dfrac{1}{x_i}-1+\sum_{j\neq i}^{c-1}\left(\dfrac{M_j}{M_c}-1\right)\dfrac{x_j}{x_i}\right\}}$	w_i	$\dfrac{1}{1+\dfrac{1}{m_iM_i}\left(1+\sum_{j\neq i}^{c-1}m_jM_j\right)}$	$\dfrac{c_iM_i}{\rho}$
$m_i=$	$\dfrac{1}{M_c\left(\dfrac{1}{x_i}-1-\sum_{j\neq i}^{c-1}\dfrac{x_j}{x_i}\right)}$	$\dfrac{1}{M_i\left(\dfrac{1}{w_i}-1-\sum_{j\neq i}^{c-1}\dfrac{w_j}{w_i}\right)}$	m_i	$\dfrac{1}{\dfrac{1}{c_i}\left(\rho-\sum_{j\neq i}^{c-1}c_jM_j\right)-M_i}$
$c_i=$	$\dfrac{\rho}{M_i+M_c\left\{\dfrac{1}{x_i}-1+\sum_{j\neq i}^{c-1}\left(\dfrac{M_j}{M_c}-1\right)\dfrac{x_j}{x_i}\right\}}$	$\dfrac{\rho w_i}{M_i}$	$\dfrac{\rho}{\dfrac{1}{m_i}\left(1+\sum_{j\neq i}^{c-1}m_jM_j\right)+M_j}$	c_i

follow, where possible, IUPAC *Green Book*.[3] A few quantities follow the ISO standards[8] or the German standard;[9] see a review by Cvitas[10] for details.

A note on nomenclature

The nomenclature of the IUPAC *Green Book*[3] 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*.

1. *Mole fraction* of substance 1, x_1 or x (1) (condensed phases), y_1 (gases):

$$x_1=n_1\Big/\sum_{s=1}^{c}n_s \tag{1}$$

where n_s is the amount of substance of s, and c is the number of distinct substances present (often the number of thermodynamic components in the system). *Mole percent* of substance 1 is 100 x_1.

2. *Ionic mole fractions* of salt i, x_{i+}, x_{i-}:
For a mixture of s binary salts i, each of which ionizes completely into ν_{s+} cations and ν_{s-} anions, with $\nu_s=\nu_{s+}+\nu_{s-}$ and a mixture of p nonelectrolytes j, of which some may be solvent components, a generalization of the definition in Ref. 11 gives

$$x_{i+}=\frac{\nu_i+x_i}{1+\sum_{i=1}^{s}(\nu_i-1)x_s},\quad x_{i-}=\frac{\nu_i-x_{i+}}{\nu_{i+}}\quad i=1\ldots s \tag{2}$$

$$x_j'=\frac{x_j}{1+\sum_{i=1}^{s}(\nu_i-1)x_i},\quad j=(s+1),\ldots,p. \tag{3}$$

The sum of these mole fractions is unity, so that, with $c=s+p$,

$$\sum_{i=1}^{s}(x_{i+}+x_{i-})+\sum_{i=s+1}^{c}x_i'=1. \tag{4}$$

General conversions to other units in multicomponent systems are complicated. For a three-component system containing nonelectrolyte 1, electrolyte 2, and solvent 3,

$$x_1=\frac{\nu_{2+}x_1'}{\nu_{2+}-(\nu_2-1)x_{2+}},\quad x_2=\frac{x_{2+}}{\nu_{2+}-(\nu_2-1)x_{2+}}. \tag{5}$$

These relations are used in solubility equations for salts, and for tabulation of salt effects on solubilities of gases (see below).

3. *Mass fraction* of substance 1, w_1 or $w(1)$:

$$w_1=g_1\Big/\sum_{s=1}^{c}g_s \tag{6}$$

where g_s is the mass of substance s. *Mass percent* of substance 1 is 100 w_1. The equivalent terms *weight fraction, weight percent,* and *g(1)/100 g solution* are no longer used.

4. *Molality* of solute 1 in a solvent 2, m_1:

$$m_1=n_1/n_2M_2 \tag{7}$$

SI base units: mol kg^{-1}. Here, M_2 is the molar mass of the solvent.

5. *Aquamolality, Solvomolality* of substance 1 in a mixed solvent with components, 2, 3,[12] $m_1^{(3)}$:

$$m_1^{(3)}=m_1\overline{M}/M_3 \tag{8}$$

SI base units: mol kg^{-1}. Here, the average molar mass of the solvent is

$$\overline{M}=x_2'M_2+(1-x_2')M_3 \tag{9}$$

and x_2' is the solvent mole fraction of component 2. This term is used most frequently in discussing comparative solubilities in water (component 2) and heavy water (component 3) and in their mixtures.

6. *Amount concentration* if solute 1 in a solution of volume V, c_1:

$$c_1=[\text{formula of solute}]=n_1/V \tag{10}$$

SI base units: mol m^{-3}. The symbol c_1 is preferred to [formula of solute], but both are used. The old terms *molarity*, *molar*, and *moles per unit volume* are no longer used.

7. *Mass concentration* of solute 1 in a solution of volume V, r_1: SI base units: kg m^{-3}.

$$\rho_1=g_1/V. \tag{11}$$

8. *Mole ratio*, $r_{\mathrm{A,B}}$ (dimensionless)[10]

$$r_{\mathrm{A,B}}=n_1/n_2. \tag{12}$$

Mass ratio, symbol $\zeta_{\mathrm{A,B}}$, may be defined analogously.[10]

Mole and mass fractions are appropriate to either the mixture or the solution point of view. The other quantities are appropriate to the solution point of view only. Conversions between pairs of these quantities can be carried out using the equations given in Table 1 at the end of this Introduction. Other useful quantities will be defined in the prefaces to individual volumes or on specific data sheets.

9. *Density*, ρ:

$$\rho=g/V \tag{13}$$

SI base units: kg m^{-3}. Here g is the total mass of the system.

10. *Relative density*, $d=\rho/\rho°$: the ratio of the density of a mixture at temperature t, pressure p to the density of a reference substance at temperature t', pressure p'. For liquid solutions, the reference substance is often water at 4 °C, 1 bar. (In some cases 1 atm is used instead of 1 bar.) The term *specific gravity* is no longer used.

Thermodynamics of Solubility

Thermodynamic analysis of solubility phenomena provides a rational basis for the construction of functions to represent solubility data, and thus aids in evaluation, and sometimes enables thermodynamic quantities to be extracted. Both these aims are often difficult to achieve because of a lack of experimental or theoretical activity coefficients. Where thermodynamic quantities can be found, they are not evaluated critically, since this task would involve examination of a large body of data that is not directly relevant to solubility. Where possible, procedures for evaluation are based on established thermodynamic methods. Specific procedures used in a particular volume will be described in the Preface to this volume.

2.4. References for the Introduction

[1] E. A. Hill, J. Am. Chem. Soc. **22**, 478 (1990).

[2] IUPAC Commission on Atomic Weights and Isotopic Abundances, Pure Appl. Chem. **63**, 975 (1980).

[3] I. Mills *et al.*, eds., *Quantities, Units and Symbols in Physical Chemistry* (The *Green Book*). (Blackwell Scientific Publications, Oxford, UK, 1993).

[4] H. H. Ku, p. 73; C. Eisenhart, p. 69; in H. H. Ku, ed., Precision Measurement and Calibration, *NBS Special Publication 300*, Vol. 1 (Washington, 1969).

[5] J. Regaudy and S. P. Klesney, *Nomenclature of Organic Chemistry* (IUPAC) (The *Blue Book*) (Pergamon, Oxford, 1979).

[6] V. Gold *et al.*, eds., *Compendium of Chemical Technology* (The *Gold Book*) (Blackwell Scientific Publications, Oxford, UK, 1987).

[7] H. Freiser and G. H. Nancollas, eds., *Compendium of Analytical Nomenclature* (The *Orange Book*) (The Blackwell Scientific Publications, Oxford, UK, 1987), Sect. 9.1.8.

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

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

[10] T. Cvitaŝ, Chem. Int. **17**, 123 (1995).

[11] R. A. Robinson and R. H. Stokes, *Electroyte Solutions* (Butterworths, London, 1959), 2nd ed.

[12] J. W. Lorimer, in R. Cohen-Adad and J. W. Lorimer, *Alkali Metal and Ammonium Chlorides in Water and Heavy Water (Binary Systems)*, IUPAC Solubility Data Series, Vol. 47 (Pergamon, Oxford, UK, 1991), p. 495.

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December, 1995

3. Methanol + Water

Components:
(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Propane (*n*-propane); C_3H_8; [74-98-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
K. Noda, K. Sato, K. Nagatsuka, and K. Ishida, J. Chem. Eng. Jpn. **8**, 492–3 (1975).

Variables:
T/K=273–293

Compiled by:
A. Skrzecz

3.1. Methanol + Water + Propane

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_3'	x_1''	x_2''	w_1'	w_2'	w_3'	w_1''	w_2''
		organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase			water-rich phase	
0.0	273.2	0.004	0.995	0.397	0.005	0.003	0.997	0.0002	0.537	0.009
		0.007	0.992	0.510	0.010	0.005	0.995	0.0003	0.643	0.017
		0.019	0.979	0.677	0.023	0.014	0.985	0.0008	0.772	0.036
		0.038	0.960	0.754	0.036	0.028	0.971	0.001	0.818	0.054
		0.147	0.848	0.851	0.099	0.112	0.886	0.002	0.838	0.134
20.0	293.2	0.007	0.992	0.276	0.003	0.005	0.994	0.0006	0.402	0.007
		0.015	0.983	0.458	0.010	0.011	0.988	0.0008	0.594	0.018
		0.019	0.978	0.493	0.014	0.014	0.985	0.001	0.624	0.025
		0.035	0.961	0.639	0.041	0.026	0.972	0.0015	0.730	0.064
		0.066	0.929	0.718	0.115	0.049	0.949	0.002	0.740	0.163

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used, similar to that reported in Ref. 1. Samples of each phase were analyzed by glc on a 3 mm diameter by 3 m long column packed with Poropak R and using H_2 as a carrier gas. Each sample was injected several times and the composition was determined from chromatogram areas. Care was taken to avoid contamination by the surroundings, especially water vapor.

Source and Purity of Materials:

(1) source not specified, commercially available; guaranteed reagent; used as received.
(2) Takachiho Chemical Industry Co., Ltd; standard reagent; used as received.
(3) distilled.

Estimated Error:
Not reported.

References:
[1] K. Ishida, Bull. Chem. Soc. Jpn. **29**, 956 (1956).

Components:
(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Butane (*n*-butane); C_4H_{10}; [106-97-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
K. Noda, K. Sato, K. Nagatsuka, and K. Ishida, J. Chem. Eng. Jpn. **8**, 492–3 (1975).

Variables:
T/K=273–293

Compiled by:
A. Skrzecz

3.2. Methanol + Water + Butane

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_3'	x_1''	x_2''	w_1'	w_2'	w_3'	w_1''	w_2''
		organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase			water-rich phase	
0.0	273.2	0.011	0.988	0.584	0.007	0.006	0.994	0.0003	0.707	0.015
		0.020	0.979	0.729	0.019	0.011	0.989	0.0004	0.805	0.039
		0.037	0.961	0.811	0.044	0.021	0.978	0.0006	0.834	0.082
		0.063	0.934	0.843	0.073	0.036	0.963	0.0007	0.824	0.130
		0.100	0.897	0.835	0.123	0.058	0.941	0.0008	0.772	0.206
		0.105	0.892	0.834	0.131	0.061	0.938	0.0008	0.764	0.218
20.0	293.2	0.007	0.991	0.270	0.001	0.004	0.996	0.0004	0.396	0.003
		0.014	0.984	0.510	0.005	0.008	0.991	0.0006	0.644	0.011
		0.020	0.978	0.626	0.010	0.011	0.988	0.0007	0.737	0.022
		0.023	0.974	0.650	0.013	0.013	0.986	0.0008	0.753	0.027
		0.041	0.956	0.723	0.023	0.023	0.976	0.001	0.797	0.046
		0.060	0.937	0.759	0.056	0.034	0.965	0.001	0.787	0.105
		0.082	0.914	0.783	0.092	0.047	0.951	0.0015	0.768	0.163
		0.121	0.873	0.751	0.177	0.071	0.927	0.002	0.675	0.289

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used, similar to that reported in Ref. 1. Samples of each phase were analyzed by glc on a 3 mm diam by 3 m long column packed with Poropak R and using H_2 as a carrier gas. Each sample was injected several times and the composition was determined from chromatogram areas. Care was taken to avoid contamination by the surroundings, especially water vapor.

Source and Purity of Materials:

(1) source not specified, commercially available; guaranteed reagent; used as received.
(2) Takachiho Chemical Industry Co., Ltd; standard reagent; used as received.
(3) distilled.

Estimated Error:
Not reported.

References:
[1] K. Ishida, Bull. Chem. Soc. Jpn. **29**, 956 (1956).

Components:	**Original Measurements:**
(1) Methanol (methyl alcohol); CH_4O; [67-56-1] (2) Isoprene (2-methyl-1,3-butadiene, isopentadiene); C_5H_8; [78-79-5] (3) Water; H_2O; [7732-18-5]	T. M. Lesteva, S. K. Ogorodnikov and V. I. Morozova, Zh. Prikl. Khim. (Leningrad) **39**, 2134–6 (1966). [Eng. transl. Russ. J. Phys. Appl. Chem. (Leningrad) **39**, 2002–5 (1966)].
Variables: T/K=288	**Compiled by:** A. Skrzecz

3.3. Methanol + Water + 2-Methyl-1, 3-butadiene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
15.0	288.2	0.0000	0.0002	0.0000	0.0008
		0.0595	0.0006	0.101	0.002
		0.1241	0.0006	0.201	0.002
		0.1652	0.0006	0.260	0.002
		0.2809	0.0010	0.409	0.003
		0.2709	0.0010	0.397	0.003
		0.3490	0.0010	0.487	0.003
		0.0646	0.0011	0.109	0.004
		0.1824	0.0015	0.283	0.005
		0.2768	0.0023	0.403	0.007
		0.3443	0.0037	0.479	0.011
		0.3690	0.0045	0.505	0.013
		0.4245	0.0090	0.557	0.025
		0.5098	0.0152	0.630	0.040
		0.5679	0.0227	0.671	0.057
		0.5197	0.0225	0.630	0.058
		0.5560	0.0318	0.650	0.079
		0.6050	0.0384	0.682	0.092
		0.6077	0.0393	0.683	0.094
		0.6351	0.0530	0.688	0.122
		0.6575	0.0720	0.683	0.159
		0.6653	0.0930	0.666	0.198
		0.6647	0.0936	0.665	0.199
		0.6780	0.1026	0.665	0.214
		0.6685	0.1090	0.652	0.226
		0.6694	0.1251	0.637	0.253
		0.6825	0.1346	0.637	0.267
		0.6675	0.1443	0.618	0.284
		0.6602	0.1724	0.589	0.327
		0.6434	0.1772	0.574	0.336
		0.6473	0.2106	0.551	0.381
		0.6263	0.2383	0.518	0.419
		0.5841	0.3033	0.452	0.499
		0.5807	0.3105	0.446	0.507
		0.5204	0.3991	0.368	0.600
		0.5060	0.4103	0.355	0.612
		0.4833	0.4388	0.331	0.639
		0.4546	0.4758	0.302	0.672
		0.3983	0.5478	0.250	0.731
		0.3991	0.5579	0.248	0.737
		0.3464	0.6294	0.204	0.788
		0.2448	0.7232	0.136	0.854
		0.1909	0.7957	0.101	0.895
		0.0000	0.9989	0.0000	0.9997

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
15.0	288.2	0.0000	0.9962	0.0406	0.0003	0.000	0.999	0.070	0.001
		0.0000	0.9925	0.0917	0.0006	0.000	0.998	0.152	0.002
		0.0000	0.9888	0.1551	0.0003	0.000	0.997	0.246	0.001
		0.0063	0.9899	0.1796	0.0003	0.003	0.996	0.280	0.001
		0.0063	0.9862	0.2203	0.0006	0.003	0.995	0.334	0.002
		0.0147	0.9779	0.4678	0.0081	0.007	0.991	0.600	0.022
		0.0412	0.9478	0.5592	0.0169	0.020	0.977	0.671	0.043
		0.0614	0.9314	0.5904	0.0264	0.030	0.968	0.685	0.065
		0.2587	0.7252	0.2587	0.7252	0.143	0.852	0.143	0.852[a]

[a] Critical point of solution estimated by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

The standard titration method was used to construct the binodal curve. Refractive indexes and densities of points on the binodal curve were measured. Ternary mixtures of known composition were shaken in the thermostat for 1 h. After separation, refractive indexes and densities of both phases were measured and concentrations were calculated from calibration curves prepared during solubility measurements. The results of the analysis of the water-rich phase were checked for a few points by redistillation and further analysis of distillate by glc and the Karl Fischer methods.

Source and Purity of Materials:

(1) source not specified; distilled several times on laboratory columns; purity 99.85%–99.90%.

(2) source not specified; distilled several times on laboratory columns; purity 99.85%–99.90%.

(3) not specified.

Estimated Error:

temp. ±0.1 °C.

Components:	**Evaluated by:**
(1) Methanol (methyl alcohol); CH_4O; [67-56-1] (2) Benzene: C_6H_6; [71-43-2] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.05)

3.4. Methanol + Water + Benzene

Critical Evaluation:

A survey of reported compositions along the saturation curves (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system methanol–benzene–water is given in Table 2.

TABLE 2. Summary of experimental data for the system methanol–benzene–water

Author(s), year	T/K	Type of data[a]	Ref.
Bancroft, 1895	293	sat. (8)	1
Holmes, 1918	288	sat. (1)	2
Perrakis, 1925	293	sat. (11)	3
Barbaudy, 1926	298	Eq. (3)	4
Ormandy *et al.*, 1934	288	sat. (5)	5
Sata and Niwase, 1937	292–304	sat. (15)	6
Leikola, 1940	299	sat. (8)	7
Staveley *et al.*, 1951	288–341	sat. (49)	8
Francis, 1954	295	sat. (16)	9
Udovenko and Mazanko, 1963	289–341	sat. (82), Eq. (44)	10
Bundantseva *et al.*, 1976	293	sat. (5), Eq. (10)	11
Triday, 1984	293	sat. (27), Eq. (10)	12
Letcher *et al.*, 1990	298	sat. (13), Eq. (5)	13

[a] Number of experimental points in parentheses.

Saturation curves

The ternary system methanol–benzene–water forms a miscibility gap of type 1. The system was the object of 13 studies over the temperature range 288–341 K. This critical evaluation is based on the original papers with the exception of data of Bancroft,[1] Ormandy, *et al.*,[5] and Leikola,[7] which were taken from the handbook of Kafarov;[14] these data sets were also taken into account during evaluation but are not reported as compilation sheets because they do not contribute further to knowledge of the system. Data of Perrakis[3] at 293 K show a larger miscibility gap than other studies; maximum mole fraction of methanol is larger by about 0.1 than any other data at this temperature. Data of Bancroft[1] were reported in volume % and were not recalculated. Therefore these data are rejected and are not reported as a compilation table. All experimental data of Letcher *et al.*[13] were presented only in graphical form and therefore were not reported as a separate compilation sheet. Data of Francis[9] at 295 K show a slightly smaller miscibility gap than data at 293 K (in agreement with general expectations), while data published during the period 1918–40 are all very close to the binodal curve describing saturation at 293 K, even though they were measured over the range 288–299 K. Of the three related binary systems, only benzene–water shows partially miscibility. The data for this system were reported, compiled, and critically evaluated in a previously published SDS volume.[15] The recommended values of mutual solubility at 293.2 K, from Ref. 15, are: $x_2'=0.9975$ and $x_2''=0.000\,406$. Only the papers of Budantseva *et al.*[11] and Triday[12] reported mutual solubility of the binary system. These values at 293.2 K[11] and at 293.0 K[12] are the same in both references: $x_2'=0.9974$, $x_2''=0.0004$ and are in excellent agreement with recommended data, Ref. 15. Characteristic points on the binodal curve of the system methanol–benzene–water at selected temperatures, reported in literature, are presented in Table 3. At the point of maximum methanol concentration the errors estimated by the evaluator are 0.005 and 0.015 mole fraction of methanol and benzene, respectively. The composition of plait points at 293 K reported in Refs. 11 and 12, differed by 0.04 mole fraction of methanol and benzene (the plait point reported by Triday[12] was calculated by Hand's method).[16]

TABLE 3. Characteristic points on the binodal curve of the system methanol–benzene–water

	Max. CH_3OH concentration			Plait points		
T/K	x_1	x_2	Ref.	x_1	x_2	Ref.
293.0	0.6181	0.1371	12	0.406	0.523	12
293.2	0.6320	0.1462	11	0.441	0.482	11
298.2	—	—		0.4743	0.4106	4
298.2	0.62	0.14	13	0.47	0.44	13
303.2	0.5949	0.1499	10	0.470	0.420	10
318.2	0.5662	0.1542	10	0.467	0.389	10
333.2	0.5345	0.1082	10	0.465	0.357	10

The temperature 293 K was selected for presentation of the behavior of the system. (The temperature difference between 293.2 and 293.0 K was neglected in binodal curve parameters calculations.) All together 72 experimental points on the saturation curve[11,12] (the water-rich and benzene-rich branches were treated together) were used to construct the fitting equation:

$$x_1=0.96828+0.11825\ \ln(x_2)-0.852\,77x_2-0.122\,05x_2^2.$$

The standard error of estimate was 0.0421. The compositions on the saturation curve calculated by the fitting equation are presented in the Table 4 for selected concentrations of benzene. The results of calculations (solid line) are presented graphically in Fig. 1 together with all experimental data reported at 293.2 K.

TABLE 4. Calculated compositions along the saturation curve at 293.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 406 Ref. 15	0.4294	0.5000
0.1506	0.0010	0.4145	0.5200
0.4152	0.0100	0.3993	0.5400
0.4886	0.0200	0.3839	0.5600
0.5533	0.0400	0.3682	0.5800
0.5840	0.0600	0.3523	0.6000
0.6006	0.0800	0.3361	0.6200
0.6095	0.1000	0.3197	0.6400
0.6135	0.1200	0.3031	0.6600
0.6140	0.1400	0.2864	0.6800
0.6120	0.1600	0.2694	0.7000
0.6080	0.1800	0.2522	0.7200
0.6025	0.2000	0.2348	0.7400
0.5957	0.2200	0.2172	0.7600
0.5878	0.2400	0.1995	0.7800
0.5790	0.2600	0.1816	0.8000
0.5694	0.2800	0.1635	0.8200
0.5591	0.3000	0.1452	0.8400
0.5482	0.3200	0.1268	0.8600
0.5367	0.3400	0.1082	0.8800
0.5247	0.3600	0.0895	0.9000
0.5122	0.3800	0.0706	0.9200
0.4993	0.4000	0.0515	0.9400
0.4860	0.4200	0.0323	0.9600
0.4723	0.4400	0.0130	0.9800
0.4584	0.4600	0.0032	0.9900
0.4440	0.4800	0.0000	0.9975 Ref. 15

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system methanol–benzene–water were reported in five references as 6 isotherms, Refs. 4, 10, 11, 12, 13, over the temperature range 293–333 K. The tie lines cover the full area of the miscibility gap. There is a large difference of mole fraction of methanol between the benzene-rich and water-rich phases. The reported data are consistent within each data set. Changes of tie line direction were observed with temperature. With decreasing temperature the water concentration in the benzene-poor phase also decreased for a similar composition of benzene-rich phase. This may be observed in data reported in Refs. 10, 11, 12. At 293 K equilibrium data of Budantseva *et al.*[11] and Triday[12] differ one from the other. For similar composition of benzene-rich phase the measured composition of water-rich phase reported by Triday[12] contains much more methanol than the equivalent mixture reported by Budantseva *et al.*[11] All equilibrium data are considered tentative. The experimental plait points reported in literature are presented above in Table 2. The experimental points at 293.2 K, both saturation and equilibrium data, Refs. 11 and 12, are presented in Fig. 1.

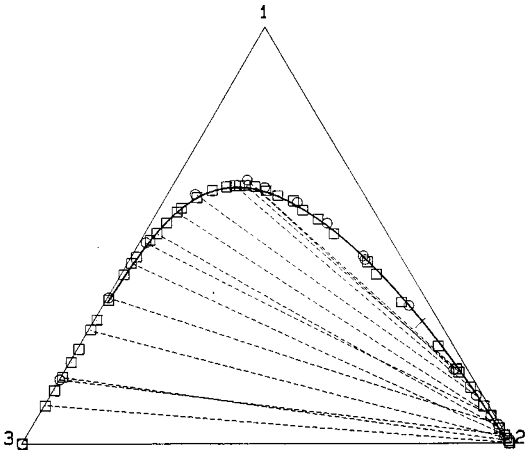

FIG. 1. Phase diagram of the system methanol (1)—benzene (2)—water (3) at 293.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 11, □—experimental data, Ref. 12, dashed lines—experimental tie lines, Refs. 11 and 12.

References:

[1] W. D. Bancroft, Phys. Rev. **3**, 205 (1895).
[2] J. Holmes, J. Chem. Soc. **113**, 263 (1918).
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[8] L. A. K. Staveley, R. G. S. Johns, and B. C. Moore, J. Chem. Soc. 2516 (1951).
[9] A. W. Francis, Ind. Eng. Chem. **46**, 205 (1954).
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[13] T. M. Letcher, J. Sewry, and S. Radloff, S. Afr. J. Chem. **43**, 56 (1990).
[14] V. V. Kafarov, ed., *Spravochnik po Rastvorimosti* Vol. 2, Troinye, Mnogokomponentnye Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskva, 1963).
[15] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).
[16] D. B. Hand, J. Phys Chem. **34**, 1961 (1930).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Benzene; C_6H_6 [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

J. Barbaudy, C. R. Hebd. Seances Acad. Sci. **182**, 1279–81 (1926).

Variables:

$T/K=298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

$t/°C$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hyrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.0925	0.8961	0.5192	0.0343	0.0405	0.9567	0.6080	0.0980
		0.0961	0.8918	0.5377	0.0409	0.0422	0.9548	0.6150	0.1140
		0.0933	0.8953	0.5240	0.0359	0.0409	0.9563	0.6100	0.1020[a]
		0.4743	0.4106	0.4743	0.4106	0.3080	0.6500	0.3080	0.6500[b]

[a] Equal density of both phases (interpolated by the author).
[b] Plait point.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. After separation, density and refractive index of each phase were measured. Compositions of coexisting phases were determined as intersections of constant density and constant refractive index lines. Nine tie lines are presented graphically. Only two of them and critical point are reported as numerical values and presented above. The procedure was described for ethanol–benzene–water system in Ref. 1.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) source not specified.

Estimated Error:

Not reported.

References:

[1] J. Barbaudy, Bull. Soc. Chim. Fr. **49**, 371 (1926).

Components:

(1) Methanol (methyl alcohol); Ch$_4$O; [67-56-1]
(2) Benzene; C_6H_6 [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

N. Sata and Y. Niwase, Bull. Chem. Soc. Jpn. **12,** 86–95 (1937).

Variables:

T/K = 292–304

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
23.0	296.2	0.4282	0.5026	0.2530	0.7240
26.0	299.2	0.4249	0.5001	0.2520	0.7230
30.0	303.2	0.4198	0.4939	0.2510	0.7200
19.0	292.2	0.4996	0.4095	0.3225	0.6445
23.5	296.7	0.4986	0.4092	0.3221	0.6444
24.0	297.2	0.4969	0.4078	0.3217	0.6436
28.0	301.2	0.4952	0.4064	0.3213	0.6428
31.0	304.2	0.4934	0.4049	0.3209	0.6419
30.0	303.2	0.4906	0.4031	0.3200	0.6410
25.5	298.7	0.5491	0.3384	0.3820	0.5740
22.0	295.2	0.5460	0.3368	0.3810	0.5730
30.0	303.2	0.5449	0.3356	0.3810	0.5720
25.0	298.2	0.6089	0.2503	0.4690	0.4700
29.0	302.2	0.6059	0.2491	0.4680	0.4690
30.0	303.2	0.6029	0.2478	0.4670	0.4680

Auxiliary Information

Method/Apparatus/Procedure:

Alcohol was added to a known amount of water–benzene mixture until one layer was obtained.

Source and Purity of Materials:

(1) Merck, ‘‘very pure,’’ without acetone; used as received.
(2) source not specified; used as received.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. A. K. Staveley, R. G. S. Johns, and B. C. Moore, J. Chem. Soc. 2516–23 (1951).

Variables:

T/K = 288–341

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
26.0	299.15	0.0113	0.985 63	0.004 68	0.994 61
33.5	306.65	0.0113	0.984 74	0.004 68	0.994 40
37.7	310.85	0.0113	0.984 08	0.004 68	0.994 24
46.1	319.25	0.0113	0.982 52	0.004 69	0.993 87
60.1	333.25	0.0113	0.979 245	0.004 70	0.993 09
20.0	293.15	0.0226	0.974 52	0.009 42	0.989 91
32.4	305.55	0.0226	0.972 89	0.009 43	0.989 51
42.0	315.15	0.0226	0.971 19	0.009 44	0.989 10
49.8	322.95	0.0226	0.968 53	0.009 46	0.988 45
56.4	329.55	0.0226	0.967 60	0.009 47	0.988 22
28.7	301.85	0.0332	0.962 65	0.013 94	0.985 08
34.5	307.65	0.0332	0.961 72	0.013 95	0.984 85
40.1	313.25	0.0332	0.960 72	0.013 96	0.984 61
47.9	321.05	0.0332	0.959 03	0.013 98	0.984 19
56.5	329.65	0.0332	0.956 62	0.014 00	0.983 58
28.4	301.55	0.0412	0.954 49	0.017 40	0.981 59
32.2	305.35	0.0412	0.954 075	0.017 41	0.981 48
44.6	317.75	0.0412	0.951 375	0.017 44	0.980 80
52.0	325.15	0.0412	0.949 68	0.017 47	0.980 37
62.8	335.95	0.0412	0.946 52	0.017 51	0.979 57
22.5	295.65	0.0458	0.950 13	0.019 37	0.979 66
41.1	314.25	0.0458	0.946 76	0.019 42	0.978 80
47.4	320.55	0.0458	0.945 03	0.019 45	0.978 36
64.1	337.25	0.0458	0.940 09	0.019 53	0.977 09
67.6	340.75	0.0458	0.939 11	0.019 54	0.976 84
23.7	296.85	0.0568	0.936 79	0.024 23	0.974 23
31.6	304.75	0.0568	0.935 31	0.024 26	0.973 85
37.9	311.05	0.0568	0.933 89	0.024 29	0.973 47
47.8	320.95	0.0568	0.931 49	0.024 33	0.972 85
50.7	323.85	0.0568	0.930 69	0.024 35	0.972 64
22.2	295.35	0.0781	0.913 62	0.033 81	0.964 18
32.7	305.85	0.0781	0.911 27	0.033 87	0.963 53
46.2	319.35	0.0781	0.908 42	0.033 95	0.962 75
53.1	326.25	0.0781	0.906 59	0.034 00	0.962 25
61.6	334.75	0.0781	0.903 74	0.034 08	0.961 46
15.0	288.15	0.1047	0.885 86	0.046 13	0.951 53
22.2	295.35	0.1047	0.884 48	0.046 18	0.951 13
35.6	308.75	0.1047	0.880 67	0.046 33	0.950 03
43.7	316.85	0.1047	0.878 85	0.046 40	0.949 50

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Mixtures were prepared in sealed tubes; water was added from a weighed pipette to a known mass of alcohol–benzene mixture.

Source and Purity of Materials:

(1) source not specified; dried by refluxing over freshly ignited lime, and then with magnesium, distilled.
(2) source not specified; chemically purified, crystallized, distilled, dried over phosphoric anhydride.
(3) not specified.

Estimated Error:
composition <0.2%; temp. <0.2 °C.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. W. Francis, Ind. Eng. Chem. **46**, 205–7 (1954).

Variables:
$T/K = 295$

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
22	295	0.120	0.001	0.195	0.005
		0.244	0.004	0.360	0.015
		0.407	0.011	0.535	0.035
		0.524	0.036	0.610	0.102
		0.561	0.052	0.620	0.140
		0.585	0.072	0.613	0.185
		0.599	0.077	0.618	0.194
		0.603	0.144	0.550	0.320
		0.589	0.205	0.489	0.415
		0.574	0.254	0.445	0.480
		0.474	0.411	0.308	0.650
		0.356	0.565	0.200	0.775
		0.253	0.678	0.130	0.850
		0.161	0.794	0.076	0.912
		0.112	0.868	0.050	0.945
		0.094	0.894	0.041	0.956

Auxiliary Information

Method/Apparatus/Procedure:

The experimental procedure was not reported. Temperature was reported to be in the range 21–23 °C. Data were presented as a part of quaternary data of methanol–benzene–aniline–water system.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) source not specified.

Estimated Error:
temp. ±1 °C.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. V. Udovenko and T. F. Mazanko, Zh. Fiz. Khim. **37**, 2324–7 (1963).

Variables:

T/K=289–341

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
25.79	298.94	0.2862	0.6652	0.1479	0.8380
30.42	303.57	0.2849	0.6622	0.1477	0.8369
40.55	313.70	0.2831	0.6582	0.1474	0.8354
46.52	319.67	0.2816	0.6544	0.1472	0.8340
56.60	329.75	0.2791	0.6486	0.1468	0.8318
63.20	336.35	0.2773	0.6446	0.1465	0.8303
25.00	298.15	0.4065	0.5001	0.2422	0.7265
29.89	303.04	0.4036	0.4966	0.2416	0.7248
38.63	311.78	0.3973	0.4889	0.2403	0.7210
49.00	322.15	0.3886	0.4783	0.2385	0.7156
60.78	333.93	0.3806	0.4684	0.2368	0.7104
21.27	294.42	0.5579	0.2973	0.4090	0.5313
26.42	299.57	0.5532	0.2947	0.4076	0.5294
36.80	309.95	0.5419	0.2887	0.4041	0.5249
46.25	319.40	0.5323	0.2836	0.4011	0.5209
52.52	325.67	0.5199	0.2770	0.3971	0.5157
61.09	334.24	0.5065	0.2698	0.3926	0.5099
23.20	296.35	0.5844	0.2304	0.4675	0.4492
31.20	304.35	0.5734	0.2260	0.4635	0.4453
40.24	313.39	0.5597	0.2206	0.4584	0.4404
46.28	319.43	0.5495	0.2166	0.4545	0.4367
54.41	327.56	0.5341	0.2105	0.4485	0.4309
63.81	336.96	0.5168	0.2037	0.4415	0.4242
24.18	297.33	0.6028	0.1828	0.5157	0.3812
31.22	304.37	0.5918	0.1794	0.5111	0.3778
40.45	313.60	0.5756	0.1745	0.5042	0.3727
50.23	323.38	0.5579	0.1691	0.4965	0.3669
56.07	329.22	0.5453	0.1654	0.4908	0.3628
60.00	333.15	0.5366	0.1627	0.4868	0.3598
22.80	295.95	0.6103	0.1125	0.5866	0.2636
26.28	299.43	0.6034	0.1112	0.5830	0.2620
31.00	304.15	0.5862	0.1080	0.5739	0.2578
42.40	315.55	0.5622	0.1036	0.5607	0.2519
54.65	327.80	0.5339	0.0984	0.5445	0.2446
67.40	340.55	0.5027	0.0926	0.5258	0.2362
24.85	298.00	0.5735	0.0607	0.6186	0.1595
28.20	301.35	0.5596	0.0592	0.6094	0.1572
35.15	308.30	0.5427	0.0574	0.5980	0.1542
47.83	320.98	0.5113	0.0541	0.5761	0.1486
59.22	332.37	0.4820	0.0510	0.5548	0.1430
21.40	294.55	0.0588	0.0006	0.0998	0.0024
31.51	304.66	0.0587	0.0006	0.0997	0.0026
38.69	311.84	0.0587	0.0007	0.0997	0.0029
46.03	319.18	0.0588	0.0008	0.0997	0.0032
54.00	327.15	0.0587	0.0009	0.0996	0.0037
61.40	334.55	0.0588	0.0011	0.0996	0.0044
23.00	296.15	0.1032	0.0007	0.1695	0.0030
30.64	303.79	0.1032	0.0008	0.1694	0.0034
41.51	314.66	0.1032	0.0011	0.1693	0.0043
47.38	320.53	0.1031	0.0012	0.1692	0.0046
54.80	327.95	0.1031	0.0014	0.1691	0.0055
62.05	335.20	0.1031	0.0015	0.1690	0.0062
20.85	294.00	0.1792	0.0013	0.2786	0.0050
32.40	305.55	0.1791	0.0016	0.2783	0.0061
39.54	312.69	0.1791	0.0019	0.2780	0.0070
45.00	318.15	0.1791	0.0021	0.2778	0.0079
53.23	326.38	0.1790	0.0024	0.2775	0.0090
58.40	331.55	0.1790	0.0027	0.2772	0.0101
19.20	292.35	0.2437	0.0020	0.3623	0.0073
33.98	307.13	0.2435	0.0028	0.3613	0.0100
39.80	312.95	0.2434	0.0036	0.3603	0.0128
45.83	318.98	0.2432	0.0042	0.3595	0.0150
52.45	325.60	0.2430	0.0050	0.3584	0.0180
65.40	338.55	0.2427	0.0065	0.3565	0.0234
16.26	289.41	0.3407	0.0052	0.4725	0.0175
30.19	303.34	0.3398	0.0079	0.4682	0.0265
45.82	318.97	0.3389	0.0103	0.4643	0.0345
57.20	330.35	0.3379	0.0134	0.4595	0.0446
65.85	339.00	0.3372	0.0156	0.4562	0.0514
22.60	295.75	0.4511	0.0138	0.5742	0.0429
30.82	303.97	0.4500	0.0163	0.5697	0.0504
38.00	311.15	0.4489	0.0188	0.5653	0.0578
45.15	318.30	0.4477	0.0216	0.5605	0.0659
50.63	323.78	0.4467	0.0238	0.5567	0.0722
55.10	328.25	0.4445	0.0284	0.5487	0.0854
60.62	333.77	0.4430	0.0316	0.5433	0.0945
20.27	293.42	0.5396	0.0395	0.6184	0.1104
25.24	298.39	0.5372	0.0439	0.6106	0.1217
36.51	309.66	0.5331	0.0512	0.5979	0.1400
44.55	317.70	0.5277	0.0607	0.5817	0.1632
56.85	330.00	0.5190	0.0763	0.5565	0.1995
63.33	336.48	0.5120	0.0889	0.5372	0.2273

Compositions of coexisting phases

$t/°\mathrm{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
30	303.2	0.0133	0.9846	0.0303	0.0006	0.0055	0.9940	0.0525	0.0025
		0.0228	0.9730	0.0589	0.0007	0.0095	0.9895	0.1000	0.0030
		0.0345	0.9592	0.1088	0.0008	0.0145	0.9840	0.1780	0.0030
		0.0459	0.9457	0.1738	0.0016	0.0195	0.9785	0.2710	0.0060
		0.0595	0.9301	0.2712	0.0040	0.0255	0.9720	0.3940	0.0140
		0.0739	0.9138	0.3631	0.0082	0.0320	0.9650	0.4930	0.0270
		0.0913	0.8965	0.4460	0.0170	0.0400	0.9570	0.5650	0.0525
		0.1104	0.8756	0.5049	0.0311	0.0490	0.9475	0.6000	0.0900
		0.1186	0.8655	0.5432	0.0482	0.0530	0.9430	0.6100	0.1320
		0.1328	0.8495	0.5734	0.0742	0.0600	0.9355	0.6020	0.1900
		0.2167	0.7502	0.5938	0.1123	0.1050	0.8860	0.5750	0.2650
		0.2297	0.7305	0.5949	0.1499	0.1130	0.8760	0.5390	0.3310
		0.3671	0.5692	0.5599	0.2622	0.2050	0.7750	0.4310	0.4920
		0.4696	0.4197	0.4696	0.4197	0.3020	0.6580	0.3020	0.6580[a]
45	318.2	0.0145	0.9813	0.0273	0.0006	0.0060	0.9930	0.0475	0.0025
		0.0227	0.9709	0.0589	0.0007	0.0095	0.9890	0.1000	0.0030
		0.0356	0.9560	0.1103	0.0013	0.0150	0.9830	0.1800	0.0050
		0.0491	0.9363	0.1684	0.0024	0.0210	0.9755	0.2630	0.0090
		0.0646	0.9149	0.2611	0.0056	0.0280	0.9670	0.3800	0.0200
		0.0862	0.8896	0.3130	0.0082	0.0380	0.9560	0.4380	0.0280
		0.1110	0.8575	0.4030	0.0154	0.0500	0.9420	0.5250	0.0490
		0.1290	0.8360	0.4317	0.0187	0.0590	0.9320	0.5490	0.0580
		0.1326	0.8287	0.4856	0.0341	0.0610	0.9290	0.5790	0.0990
		0.1559	0.8023	0.5133	0.0466	0.0730	0.9160	0.5870	0.1300
		0.2059	0.7501	0.5518	0.0921	0.1000	0.8880	0.5650	0.2300
		0.2727	0.6753	0.5662	0.1542	0.1400	0.8450	0.5150	0.3420
		0.3607	0.5634	0.5507	0.2467	0.2030	0.7730	0.4350	0.4750
		0.4670	0.3893	0.4670	0.3893	0.3120	0.6340	0.3120	0.6340[a]
60	333.2	0.0144	0.9729	0.0212	0.0007	0.0060	0.9910	0.0370	0.0030
		0.0238	0.9635	0.0560	0.0012	0.0100	0.9870	0.0950	0.0050
		0.0491	0.9343	0.1038	0.0015	0.0210	0.9750	0.1700	0.0060
		0.0534	0.9259	0.1614	0.0026	0.0230	0.9720	0.2530	0.0100
		0.0751	0.8965	0.2187	0.0046	0.0330	0.9600	0.3280	0.0170
		0.0899	0.8781	0.2978	0.0087	0.0400	0.9520	0.4200	0.0300
		0.1065	0.8580	0.3344	0.0123	0.0480	0.9430	0.4570	0.0410
		0.1082	0.8525	0.3764	0.0178	0.0490	0.9410	0.4950	0.0570
		0.1303	0.8273	0.4250	0.0262	0.0600	0.9290	0.5330	0.0800
		0.1866	0.7618	0.4706	0.0417	0.0900	0.8960	0.5560	0.1200
		0.2220	0.7242	0.4900	0.0540	0.1100	0.8750	0.5580	0.1500
		0.2380	0.7021	0.5186	0.0747	0.1200	0.8630	0.5580	0.1960
		0.2668	0.6615	0.5346	0.1082	0.1390	0.8400	0.5350	0.2640
		0.3610	0.5239	0.5271	0.1948	0.2120	0.7500	0.4550	0.4100
		0.4099	0.4615	0.5020	0.2607	0.2550	0.7000	0.3950	0.5000
		0.4648	0.3566	0.4648	0.3566	0.3240	0.6060	0.3240	0.6060[a]

[a] Critical point of solubility.

Auxiliary Information

Method/Apparatus/Procedure:

Solubility was measured by Alekseev's method.[1] Seven solubility temperature curves of constant alcohol–benzene ratio and another seven curves of constant alcohol–water ratio were constructed. Phase equilibrium was determined by comparison of density with calibration curves obtained for saturation solutions. Critical points of solubility were obtained by Alekseev's method.[1]

Source and Purity of Materials:

(1) source not specified; b.p = 63.85 °C at 750 Torr, $d(30\ °\mathrm{C}, 4\ °\mathrm{C}) = 0.7832$, $n(25\ °\mathrm{C}, \mathrm{D}) = 1.3267$.
(2) source not spcified; b.p. = 79.00 °C at 752 Torr, $d(30\ °\mathrm{C}, 4\ °\mathrm{C}) = 0.8680$, $n(25\ °\mathrm{C}, \mathrm{D}) = 1.4980$.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Gornyi Zh. **2**, 385 (1885).

Components:
(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **438-76**, 1–12 (1976).

Variables:
T/K = 293

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
20	293.2	0.331	0.626	0.176	0.811
		0.450	0.474	0.273	0.701
		0.528	0.362	0.359	0.599
		0.578	0.276	0.434	0.505
		0.614	0.191	0.516	0.392

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
20	293.2	0.0000	0.9974	0.0000	0.0004	0.0000	0.9994	0.0000	0.0017
		0.0192	0.9782	0.1538	0.0003	0.0080	0.9914	0.2441	0.0012
		0.0450	0.9508	0.3498	0.0015	0.0190	0.9800	0.4871	0.0051
		0.0674	0.9243	0.4814	0.0128	0.0290	0.9690	0.6040	0.0392
		0.1145	0.8711	0.5972	0.0560	0.0510	0.9454	0.6430	0.1470
		0.1775	0.7941	0.6320	0.1462	0.0834	0.9091	0.5678	0.3202
		0.4410	0.4820	0.4410	0.4820	0.2658	0.7081	0.2658	0.7081[a]

[a] Critical point of solubility.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. The synthetic method was used to determine phase equilibria. The mole fraction of hydrocarbon in the charge before separation was about 0.30. After separation phases were analyzed by glc to determine methanol and hydrocarbon; concentration of water was determined by the Karl Fischer method.

Source and Purity of Materials:
(1) source not specified.
(2) source not specified; distilled; purity > 99.9%.
(3) not specified.

Estimated Error:
Not reported.

Components:
(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
J. O. Triday, J. Chem. Eng. Data **29**, 321–4 (1984).

Variables:
T/K = 293

Compiled By:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
24.8	293.0	0.0000	0.0004	0.0000	0.0017
		0.1277	0.0025	0.2050	0.0098
		0.1956	0.0028	0.2995	0.0105
		0.2271	0.0029	0.3404	0.0106
		0.2973	0.0042	0.4246	0.0146
		0.3445	0.0047	0.4772	0.0159
		0.4055	0.0055	0.5406	0.0179
		0.4473	0.0105	0.5751	0.0329
		0.4867	0.0187	0.6006	0.0563
		0.5284	0.0316	0.6196	0.0903
		0.5644	0.0443	0.6325	0.1210
		0.5896	0.0632	0.6280	0.1641
		0.6063	0.0862	0.6128	0.2124
		0.6151	0.1117	0.5909	0.2616
		0.6181	0.1371	0.5671	0.3066
		0.6060	0.1977	0.5057	0.4022
		0.5940	0.2282	0.4751	0.4450
		0.5816	0.2665	0.4417	0.4934
		0.5595	0.2965	0.4104	0.5302
		0.5378	0.3386	0.3754	0.5761
		0.5025	0.3880	0.3328	0.6264
		0.4357	0.4897	0.2607	0.7142
		0.3392	0.6072	0.1834	0.8003
		0.2884	0.6698	0.1483	0.8396
		0.2337	0.7341	0.1145	0.8767
		0.0895	0.8992	0.0391	0.9581
		0.0000	0.9974	0.0000	0.9994

Compositions of coexisting phases

$t/°C$ (compiler)	T/K	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
24.8	293.0	0.0007	0.9967	0.0914	0.0020	0.0003	0.9991	0.1508	0.0080
		0.0055	0.9915	0.1603	0.0026	0.0023	0.9970	0.2515	0.0099
		0.0114	0.9852	0.2734	0.0036	0.0047	0.9945	0.3970	0.0127
		0.0199	0.9760	0.4322	0.0073	0.0083	0.9908	0.5649	0.0233
		0.0371	0.9574	0.5033	0.0245	0.0156	0.9831	0.6075	0.0721
		0.0667	0.9249	0.5547	0.0400	0.0287	0.9693	0.6303	0.1108
		0.1339	0.8500	0.6182	0.1279	0.0604	0.9355	0.5763	0.2907
		0.1708	0.8080	0.6187	0.1496	0.0793	0.9151	0.5556	0.3275
		0.1789	0.7986	0.6161	0.1698	0.0837	0.9104	0.5355	0.3598
		0.406	0.523	0.406	0.523	0.2359	0.7409	0.2359	0.7409[a]

[a] Author's plait point.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine the binodal curve. Binary homogeneous samples of known composition were titrated in a thermostated glass-stoppered bottle with the small portions of the third component from Kimax microburette (with an accuracy of 0.01 cm^3). The mass of the titrant was calculated from its volume and density. Liquid–liquid equilibrium was measured in the thermostated cell of 250 cm^3 capacity with magnetic stirrer for the mixtures resulting equal volumes of both phases. After separation, both phases were analyzed by measuring the refractive indexes and comparing results with a calibration curve obtained earlier for saturated mixtures. Plait point was calculated by the author by the Hand's method.[1]

Source and Purity of Materials:

(1) AnalaR; distilled in a high-efficiency packed column; $\rho(293\ K)/(g\ cm^{-3}) = 0.7911$, $n(293\ K) = 1.3290$.
(2) Merck, analytical-grade; certificated purity $> 99.5\%$; used as received; $\rho(293\ K)/(g\ cm^{-3}) = 0.8790$, $n(293\ K) = 1.5011$.
(3) de-ionized and distilled.

Estimated Error:

temp. ±0.1 K; composition ±0.0005 mole fraction.

References:

[1] D. B. Hand, J. Phys. Chem. **34**, 1961 (1930).

Components:
(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Cyclohexene; C_6H_{10}; [110-83-8]
(3) Water; H_2O; [7732-18-5]

Evaluated by:
A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.04)

3.5. Methanol + Water + Cyclohexene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system methanol–cyclohexene–water is given in Table 5.

TABLE 5. Summary of experimental data for the system methanol–cyclohexene–water

Author(s)	T/K	Type of data[a]	Ref.
Washburn *et al.*, 1940	298	sat. (16), eq. (7)	1
Budantseva *et al.*, 1976	293	sat. (6), eq. (9)	2

[a] Number of experimental points in parentheses.

Saturation curve

The system methanol–cyclohexene–water forms a large miscibility gap of type 1 covering the majority of the concentration triangle. Compositions along the saturation curves reported in both references were obtained by the titration method. Experimental data within each data set, measured at various temperatures, as well as between data sets, are consistent. Only one binary system, cyclohexene–water, forms miscibility gap. Binary data of this system were compiled and critically evaluated in a previously published SDS volume.[3] The recommended, Ref. 3, values of mutual solubility at 298 K are: $x'_2 = 0.9983$ and $x''_2 = 0.000\ 035$. Budantseva *et al.*[2] report data of mutual solubility at 293.2 K which are almost equal $x'_2 = 0.9981$, $x''_2 = 0.000\ 05$. The saturation curves for both temperatures are located very closely to one to another, a temperature difference 5 K is not significant. Maximum methanol concentration on saturation curve is observed at the region close to $x_1 = 0.78$, $x_2 = 0.14$. All experimental data, reported at 293 and 298 K in the two references are treated as tentative.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system methanol–cyclohexene–water were reported in both references. After separation, phases in equilibrium were analyzed. Washburn *et al.* [1] reported that the hydrocarbon-rich phase did not contain water, which presumably was the result of analytical limitations (self constructed refractive index–composition curve). Budantseva *et al.*[2] used more precise analytical methods (glc—for methanol and cyclohexene and the Karl Fischer—for water). Their results seem more reliable. The plait point of the system reported at 293.2 K,[1] was $x_1 = 0.504$, $x_2 = 0.477$. The miscibility gap of the binary cyclohexene–methanol system may exist at temperatures below 270 K, but this region was not studied in Ref. 4. The equilibrium data are treated as tentative. Experimental data of Budantseva *et al.*[2] at 293.2 K are presented in Fig. 2.

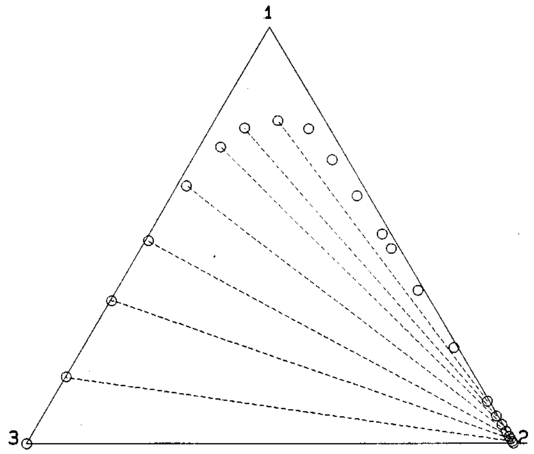

FIG. 2. Phase diagram of the system methanol (1)—cyclohexene (2)—water (3) at 293.2 K. ○—experimental data, Ref. 2, dashed lines—experimental tie lines, Ref. 2.

References:

[1] E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transue, J. Am. Chem. Soc. **62**, 1454 (1940).

[2] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **438-76**, 1 (1976).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[4] D. G. Shaw, A. Skrzecz, J. W. Lorimer, and A. Maczynski, eds., *Solubility Data Series*, Vol. 56, Alcohols with Hydrocarbons (Pergamon, New York, 1994).

Components:

(1) Methanol (mel alcohol); CH_4O; [67-56-1]
(2) Cyclohexene; C_6H_{10} ; [110-83-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transue, J. Am. Chem. Soc. **62**, 1454–7 (1940)

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.15	0.2372	0.7585	0.1086	0.8903
		0.3974	0.5937	0.2065	0.7909
		0.5341	0.4514	0.3143	0.6809
		0.6426	0.3366	0.4235	0.5688
		0.7308	0.2317	0.5430	0.4413
		0.7866	0.1397	0.6631	0.3020
		0.7761	0.0731	0.7404	0.1787
		0.7333	0.0401	0.7611	0.1067
		0.6709	0.0231	0.7436	0.0657
		0.6007	0.0117	0.7079	0.0352
		0.5175	0.0064	0.6456	0.0205
		0.4196	0.0025	0.5587	0.0087
		0.3429	0.0013	0.4796	0.0048
		0.2497	0.0005	0.3712	0.0020
		0.1574	0.0002	0.2492	0.0010
		0.0923	0.0001	0.1531	0.0005

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.15	0.0026	0.9974	0.0563	0.0000	0.001	0.999	0.096	0.000
		0.0051	0.9949	0.1086	0.0002	0.002	0.998	0.178	0.001
		0.0051	0.9949	0.1723	0.0002	0.002	0.998	0.270	0.001
		0.0077	0.9923	0.2018	0.0003	0.003	0.997	0.310	0.001
		0.0102	0.9898	0.2734	0.0008	0.004	0.996	0.400	0.003
		0.0302	0.9698	0.6373	0.0171	0.012	0.988	0.728	0.050
		0.0521	0.9479	0.7252	0.0372	0.021	0.979	0.760	0.100

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, as described in Ref. 1, was used. The titrant, from a weighed pipette, was added to the weighed binary mixture of known composition and the mixture was kept in a thermostated bath. To confirm that the end-point was reached the mixture was shaken automatically for at least 15 min and then reexamined. The plot of refractive index against composition was then used to find compositions of equilibrium phases. The refractive indexes were determined at the temperature of 30.0 °C to eliminate an opalescence.

Source and Purity of Materials:

(1) Eastman Kodak Company, commercial grade; dried by refluxing over active lime, twice distilled; $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.7866$, $n(25\ °\mathrm{C,D})=1.326\ 59$.
(2) Eastman Kodak Company, commercial grade; distilled in an atmosphere of purified N_2, collected in dried nitrogen-filled bottles; $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.8056$, $n(25\ °\mathrm{C,D})=1.4434$.
(3) not specified.

Estimated Error:

temp. ±0.05 °C.

References:

[1] E. R. Washburn and A. E. Beguin, J. Am. Chem. Soc. **62**, 579 (1940).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Cyclohexene; C_6H_{10} ; [110-83-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **438–76**, 1–12 (1976).

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
20	293.2	0.230	0.761	0.105	0.892
		0.368	0.618	0.188	0.808
		0.469	0.513	0.261	0.733
		0.595	0.380	0.376	0.615
		0.680	0.287	0.474	0.513
		0.754	0.202	0.582	0.399

Compositions of coexisting phases

		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
20	293.2	0.0000	0.9981	0.0000	0.00005	0.0000	0.9996	0.0000	0.00023
		0.0045	0.9937	0.1603	0.0005	0.0018	0.9978	0.2531	0.0020
		0.0103	0.9877	0.3437	0.0019	0.0040	0.9955	0.4797	0.0068
		0.0165	0.9813	0.4885	0.0058	0.0065	0.9930	0.6202	0.0189
		0.0284	0.9690	0.6185	0.0190	0.0113	0.9881	0.7101	0.0559
		0.0447	0.9522	0.7107	0.0435	0.0180	0.9813	0.7400	0.1161
		0.0655	0.9306	0.7561	0.0700	0.0267	0.9724	0.7317	0.1737
		0.1004	0.8945	0.7736	0.1295	0.0419	0.9569	0.6669	0.2862
		0.5040	0.4770	0.5040	0.4770	0.2901	0.7038	0.2901	0.7038[a]

[a] Critical point of solubility.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. The synthetic method was used to determine phase equilibria. The mole fraction of hydrocarbon in the charge before separation was about 0.30. After separation phases were analyzed by glc to determine methanol and hydrocarbon; concentration of water was determined by the Karl Fischer method.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified; distilled; purity > 99.9%.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Cyclohexane; C_6H_{10} ; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.04)

3.6. Methanol + Water + Cyclohexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of methanol between phases (dist.) for the system methanol–cyclohexane–water is given in Table 6.

TABLE 6. Summary of experimental data for the system methanol–cyclohexane–water

Author(s)	T/K	Type of data[a]	Ref.
Washburn and Spencer, 1934	298	sat. (16), dist. (6)	1
Budantseva *et al.*, 1976	293	eq. (10)	2
Letcher *et al.*, 1991	298	sat. (12), eq. (3)	3
Plackov and Stern, 1992	298	sat. (14), eq. (7)	4

[a] Number of experimental points in parentheses.

Saturation curves

The system methanol–cyclohexane–water forms a large miscibility gap of type 2 covering the majority of the concentration triangle. Two binary systems, cyclohexane–water and cyclohexane–methanol, form miscibility gaps. The data of these binary systems were compiled and critically evaluated in previously published SDS volumes, Refs. 5 and 6, respectively. The recommended values[5] of mutual solubility of the cyclohexane–water system at 298.2 K are: $x_2''=1.2\cdot 10^{-5}$ and $x_3'=3.7\cdot 10^{-4}$. The mutual solubility at 298.2 K and upper critical solubility temperature of the methanol–cyclohexane system calculated on the basis of Ref. 6 are: $x_1'=0.128$ and $x_1''=0.822$ and 318.7 K. Reported data on the saturation curves describe mainly the cyclohexane-poor phase; there are few experimental points in the cyclohexane-rich region. Data for both temperatures are in agreement with one another with the exception of the Washburn and Spencer data[1] in the cyclohexane-rich phase, which presents too high concentration of water. All experimental solubility and equilibrium data at 298 K in cyclohexane-poor phase[1,3,4] were described by the equation:

$$x_1=1.07468+0.05543\ \ln(x_3)-1.07833x_3\ .$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0030. The equation is valid in the region of $0.02<x_3<0.50$. The points on the saturation curve calculated by the above equation for the selected concentrations of water in the mixture together with the recommended data of binary systems are presented in Table 7 and in Fig. 3 as solid line.

TABLE 7. Calculated compositions along the saturation curve at 298.2 K

x_1	x_3	x_1	x_3
0.822	0.178 Ref. 6	0.6844	0.3000
0.8363	0.0200	0.6665	0.3200
0.8531	0.0400	0.6483	0.3400
0.8540	0.0600	0.6299	0.3600
0.8484	0.0800	0.6113	0.3800
0.8392	0.1000	0.5926	0.4000
0.8278	0.1200	0.5737	0.4200
0.8147	0.1400	0.5547	0.4400
0.8006	0.1600	0.5356	0.4600
0.7855	0.1800	0.5164	0.4800
0.7698	0.2000	0.4971	0.5000
0.7535	0.2200	0.0000	0.999988 Ref. 5
0.7368	0.2400	0.0000	0.00037 Ref. 5
0.7197	0.2600	0.128	0.0000 Ref. 6
0.7022	0.2800		

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system methanol–cyclohexane–water were reported in Refs 2, 3, and 4. In Ref. 1 the distribution of methanol between two phases (hydrocarbon-rich and hydrocarbon-poor) was reported. The lines reported by Letcher *et al.*[3] were measured at the pressure of 94.7 kPa, but the influence of such pressure difference (6.6 kPa) on liquid–liquid equilibria may be neglected. The experimental tie lines of Budantseva *et al.*, Ref. 2, even they were measured at 293.2 K, are in agreement with tie lines of Plackov and Stern,[4] measured at a little higher temperature of 298.2 K. The three tie lines presented by Letcher *et al.*[3] were measured with the accuracy 0.01 mole fraction, as was reported in the paper and are not consistent with data of Ref. 4. Therefore data of Plackov and Stern,[4] in the opinion of evaluator, appear reliable and are considered as tentative. They are presented in Fig. 3.

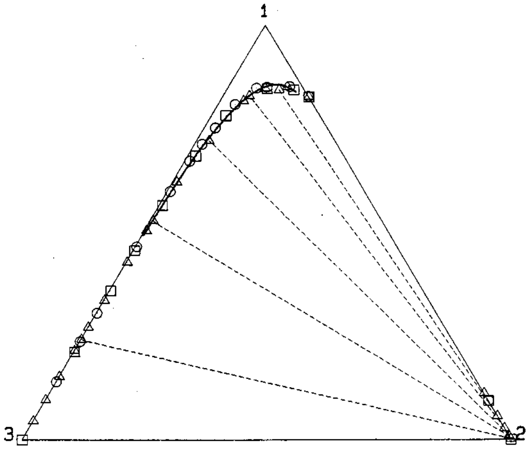

FIG. 3. Phase diagram of the system methanol (1)—cyclohexane (2)—water (3) at 298.2 K. ○—experimental data, Ref. 1, □—experimental data, Ref. 3, △—experimental data, Ref. 4, dashed lines—tie lines, Ref. 4.

References:

[1]E. R. Washburn and H. C. Spencer, J. Am. Chem. Soc. **56**, 361 (1934).

[2]L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **438–76**, 1 (1976).

[3]T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118 (1991).

[4]D. Plackov and I. Stern, Fluid. Phase Equilib. **71**, 189 (1992).

[5]D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon New York, 1989).

[6]D. G. Shaw, A. Skrzecz, J. W. Lorimer, and A. Maczynski, eds., *Solubility Data Series*, Vol. 56, Alcohols with Hydrocarbons (Pergamon, New York, 1994).

Components:	**Original Measurements:**
(1) Methanol (methyl alcohol); CH_4O; [67-56-1] (2) Cyclohexane; C_6H_{12} ; [110-82-7] (3)Water; H_2O; [7732-18-5]	E. R. Washburn and H. C. Spencer, J. Am. Chem. Soc. **56**, 361–4 (1934).
Variables: T/K=298	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
25.0	298.2	0.1398	0.0002	0.2241	0.0010
		0.2372	0.0005	0.3556	0.0019
		0.3058	0.0008	0.4383	0.0031
		0.4663	0.0025	0.6043	0.0086
		0.5979	0.0056	0.7156	0.0176
		0.6699	0.0100	0.7645	0.0301
		0.7106	0.0151	0.7857	0.0437
		0.7504	0.0219	0.8018	0.0614
		0.8072	0.0340	0.8188	0.0906
		0.8464	0.0580	0.8041	0.1448
25.0	298.2	0.8491	0.0780	0.7754	0.1872
		0.8501	0.1237	0.7145	0.2731
		0.8264	0.1736	0.6445	0.3555
		0.0935	0.9065	0.0378	0.9622
		0.0395	0.9406	0.0157	0.9799
		0.0233	0.9683	0.0091	0.9891

Distribution of methanol in methanol–cyclohexane–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_1'' water-rich phase
25.0	298.2	0.0005	0.032
		0.0025	0.151
		0.0040	0.268
		0.0050	0.349
		0.0065	0.388
		0.0070	0.418

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to obtain points on the saturation curve. A flask containing weighted amounts of two liquids was suspended in a temperature controlled water bath and the third liquid added by means of a glass dropper which was thrust through a cork stopper. The flask was shaken after each addition of the third liquid and sufficient time allowed for equilibrium to be reached. In order to ensure complete saturation near the end-point, the bath was warmed a few tenths of a degree so that complete solution occurred and then cooled to 24.8 °C. The refractive index of each saturated mixture was measured. The tie lines were determined as recorded in Refs. 1 and 2. Refractive indexes and concentrations of methanol in phases in equilibrium were reported in the paper.

Source and Purity of Materials:

(1) synthetic from Merck Co.; refluxed over freshly ignited lime, distilled, $d(25\ °C,4\ °C)=0.786\ 73$, $n(25\ °C,D)=1.326\ 60$.
(2) Eastman Kodak Co., ''best grade;'' crystallized, distilled, dried over Na, distilled; $d(25\ °C,4\ °C)=0.773\ 54$, $n(25\ °C,D)=1.423\ 70$, f.p. $=6.10$ °C.
(3) distilled.

Estimated Error:

temp. ±0.1 °C (estimated by the compiler).

References:

[1] E. R. Washburn, V. Hnizda, and R. D. Vold, J. Am. Chem. Soc. **53**, 3237 (1931).

[2] R. D. Vold and E. R. Washburn, J. Am. Chem. Soc. **54**, 4217 (1932).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **438–76**, 1–12 (1976).

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K(compiler)	hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
20	293.2	0.0000	0.999 53	0.0000	0.000 015	0.0000	0.999 90	0.0000	0.000 070
		0.0030	0.9965	0.1935	0.0000	0.0011	0.9987	0.2991	0.0002
		0.0058	0.9937	0.3605	0.0005	0.0022	0.9977	0.4999	0.0018
		0.0086	0.9909	0.4990	0.0020	0.0033	0.9966	0.6358	0.0067
		0.0130	0.9861	0.6310	0.0062	0.0050	0.9948	0.7413	0.0191
		0.0181	0.9810	0.7284	0.0130	0.0070	0.9928	0.8023	0.0376
		0.0268	0.9723	0.8000	0.0253	0.0104	0.9894	0.8293	0.0689
		0.0394	0.9597	0.8409	0.0461	0.0154	0.9844	0.8200	0.1181
		0.0798	0.9193	0.8717	0.0808	0.0320	0.9678	0.7849	0.1911
		0.1390	0.8610	0.8570	0.1430	0.0579	0.9421	0.6953	0.3047

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The mole fraction of hydrocarbon in the charge before separation was about 0.30. After separation phases were analyzed by glc to determine methanol and hydrocarbon; concentration of water was determined by the Karl Fischer method.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified; distilled; purity >99.9%.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118–21 (1991).

Variables:

$T/K = 298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$ (compiler)	T/K	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.212	0.001	0.323	0.004
		0.360	0.002	0.497	0.007
		0.457	0.003	0.595	0.010
		0.565	0.006	0.687	0.019
		0.682	0.016	0.763	0.047
		0.780	0.029	0.809	0.079
		0.845	0.080	0.770	0.191
		0.842	0.136	0.695	0.295
		0.825	0.175	0.642	0.358
		0.093	0.907	0.038	0.962
		0.000	0.999	0.0000	0.9998

Compositions of coexisting phases

$t/°C$ (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
25.0	298.2	0.025	0.974	0.323	0.001	0.010	0.990	0.458	0.004
		0.051	0.949	0.533	0.005	0.020	0.980	0.661	0.016
		0.074	0.926	0.737	0.023	0.030	0.970	0.790	0.065

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the titration method, as described in Ref. 1. The formation of a cloudy mixture was observed visually on shaking after addition of a known mass of the third component; syringes were precisely weighed. Tie line compositions were determined by the refractive index method,[2] and a complementary method using the Karl Fischer titration.[3] Measurements were made at pressure of 94.7 kPa.

Source and Purity of Materials:

(1) Merck; AR grade; refluxed with Mg and I_2, distilled; purity >99.9 mole % by glc.
(2) BDH; Gold label grade; used as received; purity >99.9 mole % by glc.
(3) not specified.

Estimated Error:

composition ± 0.005 mole fraction (binodal curve), ± 0.01 mole fraction (tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and F. W. Comings, Ind. Eng. Chem. **35**, 411 (1993).
[3] T. M. Letcher, P. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. Plackov and I. Stern, Fluid Phase Equilib. **71**, 189–209 (1992).

Variables:

$T/K = 298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
25	298.2	0.1114	0.8886	0.0456	0.9544
		0.8250	0.1750	0.6422	0.3578
		0.8495	0.1195	0.7194	0.2658
		0.8462	0.0760	0.7766	0.1832
		0.8158	0.0472	0.8023	0.1219
		0.6196	0.0091	0.7270	0.0280
		0.5050	0.0033	0.6391	0.0110
		0.4289	0.0019	0.5689	0.0066
		0.3365	0.0010	0.4729	0.0037
		0.2713	0.0005	0.3978	0.0019
		0.2149	0.0004	0.3270	0.0016
		0.1524	0.0003	0.2421	0.0013
		0.0961	0.0003	0.1589	0.0013
		0.0454	0.0002	0.0779	0.0009

Compositions of coexisting phases

$t/°C$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
25	298.2	0.0006	0.9988	0.100	0.000	0.0002	0.9996	0.165	0.000
		0.0019	0.9975	0.242	0.001	0.0007	0.9991	0.361	0.004
		0.0047	0.9948	0.369	0.001	0.0018	0.9981	0.508	0.004
		0.0064	0.9931	0.529	0.005	0.0024	0.9974	0.658	0.016
		0.0097	0.9898	0.719	0.025	0.0037	0.9962	0.774	0.071
		0.0276	0.9720	0.828	0.053	0.0107	0.9892	0.801	0.135
		0.0567	0.9430	0.843	0.106	0.0224	0.9776	0.733	0.242

Auxillary Information

Method/Apparatus/Procedure:

Binodal compositions were determined by titration with the corresponding, less-soluble component until the appearance of turbidity.[1] The analytical method was used for determination of tie-lines. This was based on refractive indexes and densities of the samples, Ref. 1, combined with the oxidation of the alcohol with an excess of potassium dichromate and determination of unreduced dichromate with $Na_2S_2O_3$. Alcohol in the organic layer was determined after extraction with water.

Source and Purity of Materials:

(1) Kemika (Zagreb); analytical grade; presumably used as received; $n = 1.3624$, $\rho(25\ °C) = 787.7\ kg/m^3$, b.p. $= 64.6\ °C$.
(2) Kemika (Zagreb); purity not specified; presumably used as received; $n = 1.4232$, $\rho(25\ °C) = 773.9\ kg/m^3$, b.p. $= 80.0\ °C$.
(3) twice distilled in the presence of $KMnO_4$.

Estimated Error:

composition < 0.0005 mass fraction, binodal, (relative); composition ± 2%, tie line.

References:

[1] D. Plackov and I. Stern, Fluid Phase Equilib. **57**, 327 (1990).

Components:	**Original Measurements:**
(1) Methanol (methyl alcohol);CH_4O; [67-56-1] (2) 1-Hexene; C_6H_{12}; [592-41-6] (3) Water; H_2O; [7732-18-5]	L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **438-76**, 1–12 (1976).
Variables: T/K=293	**Compiled by:** A. Skrzecz

3.7. Methanol + Water + 1-Hexene

Experimental Data

Compositions along the saturation curve

				w_1	w_2
t/°C	T/K (compiler)	x_1	x_2	(compiler)	
20	293.2	0.229	0.762	0.102	0.895
		0.392	0.593	0.200	0.795
		0.513	0.465	0.294	0.699
		0.614	0.357	0.392	0.598
		0.690	0.275	0.482	0.504
		0.746	0.203	0.570	0.408

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
20	293.2	0.0000	0.9984	0.0000	0.000 01	0.0000	0.999 66	0.0000	0.000 05
		0.0049	0.9937	0.1564	0.0000	0.0019	0.9978	0.2479	0.0002
		0.0120	0.9866	0.3359	0.0004	0.0046	0.9951	0.4730	0.0015
		0.0194	0.9792	0.4973	0.0021	0.0075	0.9922	0.6341	0.0070
		0.0359	0.9623	0.6227	0.0088	0.0140	0.9856	0.7300	0.0271
		0.0566	0.9407	0.7250	0.0218	0.0224	0.9770	0.7841	0.0619
		0.0830	0.9134	0.7703	0.0421	0.0334	0.9658	0.7810	0.1121
		0.1469	0.8468	0.7885	0.1038	0.0619	0.9366	0.7030	0.2431
		0.1988	0.7931	0.7736	0.1529	0.0869	0.9111	0.6359	0.3301
		0.5200	0.4580	0.5200	0.4580	0.2997	0.6932	0.2997	0.6932[a]

[a] Critical point of solubility.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. The synthetic method was used to determine phase equilibria. The mole fraction of hydrocarbon in the charge before separation was about 0.30. After separation phases were analyzed by glc to determine methanol and hydrocarbon; concentration of water was determined by the Karl Fischer method.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified; distilled; purity >99.9%.
(3) not specified.

Estimated Error:

Not reported.

Components:	**Evaluated by:**
(1) Methanol (methyl alcohol); CH_4O; [67-56-1] (2) Hexane (n-hexane); C_6H_{14}; [110-54-3] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.04)

3.8. Methanol + Water + Hexane

Critical Evaluation

A survey of reported in the literature compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system methanol–hexane–water is given in Table 8.

TABLE 8. Summary of experimental data for the system methanol–hexane–water

Author(s)	T/K	Type of data[a]	Ref.
Bonner, 1909	273	sat. (11)	1
Suhrmann and Walter, 1951	311–323	sat. (7)	2
Kogan *et al.*, 1956	283,293	Eq. (9)	3
Budantseva *et al.*, 1976	293	Eq. (10)	4

[a] Number of experimental points in parentheses.

Saturation curve

The system methanol–hexane–water forms a large miscibility gap of type 2 covering the majority of the concentration triangle. Two binary systems, hexane–water and hexane–methanol, are partially miscible at the reported temperatures. The data for these binary systems were compiled and critically evaluated in previously published SDS volumes, Refs. 5 and 6, respectively. The recommended, values[5] of mutual solubility for the hexane water system at 293.2 K are: $x_2'=0.999\ 47$ and $x_2''=2.5\cdot 10^{-6}$. The binary data reported in Ref. 4, $x_2'=0.999\ 63$ and $x_2''=3\cdot 10^{-6}$, are in very close agreement. The recommended upper critical solution temperature and mutual solubilities at 293.2 K of the methanol–hexane system calculated on the basis of Ref. 6 are: 306.8 K and $x_1'=0.210$, $x_1''=0.822$. These recommended solubilities are exactly the mean value of experimental data reported in Refs. 3 and 4 which were also used in evaluation of the binary system. Concentration differences, in mole fraction, in hexane-rich phase are about 0.03 and in hexane-poor phase—0.006 and 0.02. Measurements along the saturation curve only were reported by Bonner[1] at 273 K and Suhrmann and Walter[2] in the range 311–323 K. This last paper shows the influence of water on the upper critical solution temperature of the system methanol–hexane. In the other studies phases in equilibrium were presented which may also be treated as points on saturation curve. The data for the hydrocarbon-poor phase on the saturation curve[3,4] in the region $x_3<0.33$ were described by the equation:

$$x_1=1.08162+0.04830\ \ln(x_3)-1.09286x_3\ .$$

The least-squares method was used and the standard error of estimate was 0.0026. For the selected concentrations of water in the mixture this part of saturation curve was calculated and the results are presented in Table 9 and in Fig. 4 as solid line. The part of the saturation curve (hydrocarbon-poor branch) in the region of $x_1<0.65$ presents very low concentration of hydrocarbon and on the basis of reported papers the relationship between concentrations of methanol and hexane may be treated as linear. The maximum concentration of methanol in hexane-poor phase of saturation curve, estimated on the basis of Ref. 4, is $x_1=0.88$ and $x_2=0.08$ within an accuracy 0.01 mole fraction. The experimental points of hexane-rich branch of saturation curve contain a very small amount of water and therefore were not described (concentration of water was smaller than 0.0001 mass fraction, Ref. 3).

TABLE 9. Calculated compositions along the saturation curve at 293.2 K (hexane-poor phase)

x_1	x_3	x_1	x_3
0.210	0.0000 Ref. 6	0.8021	0.1800
0.822	0.0000 Ref. 6	0.7853	0.2000
0.8483	0.0100	0.7681	0.2200
0.8708	0.0200	0.7504	0.2400
0.8824	0.0400	0.7324	0.2600
0.8802	0.0600	0.7141	0.2800
0.8722	0.0800	0.6956	0.3000
0.8611	0.1000	0.6769	0.3200
0.8481	0.1200	0.0000	0.999 997 5 Ref. 5
0.8337	0.1400	0.0000	0.000 53 Ref. 5
0.8183	0.1600		

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system methanol–hexane–water were reported in Refs. 3 and 4 at 283.2 and 293.2 K, respectively. The phases, when equilibrium was reached, were separated and then analyzed in various ways: methanol was determined by reaction with phthalic anhydride, Ref. 3, or by glc, Ref. 4; water was determined by the Karl Fischer reaction.[3,4] The compositions of phases in equilibrium reported in both Refs. 3 and 4 are consistent with one another. They are presented in Fig. 4.

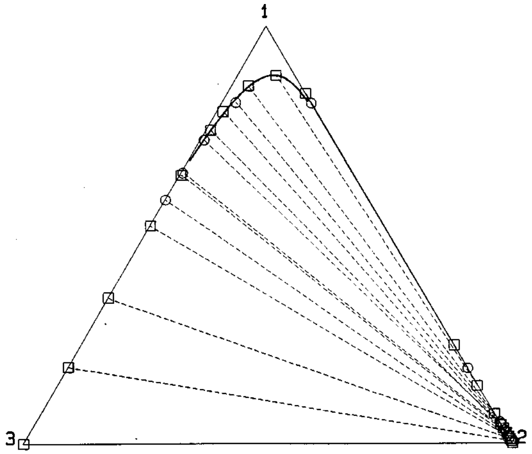

FIG. 4. Phase diagram of the system methanol (1)—hexane (2)—water (3) at 293.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 3, □—experimental data, Ref. 4, dashed lines—experimental tie lines, Refs. 3 and 4.

References:

[1] W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).

[2] R. Suhrmann and R. Walter, Abh. Braunschw. Wiss. Ges. **3**, 135 (1951).

[3] V. B. Kogan, I. V. Deizenrot, T. A. Kulbyaeva, and V. M. Fridman, Zh. Prikl. Khim (Leningrad) **29**, 1387 (1956).

[4] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsoy, Dep. Doc. VINITI **438–76**, 1 (1976).

[5] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[6] D. G. Shaw, A. Skrzecz, J. W. Lorimer, and A. Maczynski, eds., *Solubility Data Series*, Vol. 56, Alcohols with Hydrocarbons (Pergamon, New York, 1994).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910).

Variables:

$T/K=273$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)
0.0	273.2	0.9018	0.0731	0.8106	0.1767
		0.8950	0.0549	0.8358	0.1379
		0.8762	0.0394	0.8510	0.1030
		0.8674	0.0303	0.8619	0.0809
		0.8540	0.0245	0.8642	0.0667
		0.8288	0.0172	0.8619	0.0481
		0.8256	0.0163	0.8615	0.0457
		0.7857	0.0106	0.8459	0.0308
		0.7650	0.0096	0.8337	0.0283
		0.7040	0.0064	0.7964	0.0193
		0.5004	0.0017	0.6375	0.0058

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogenous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled; $n(14\,°C)=1.330\,70$.
(2) Kahlbaum; presumably dried and distilled; $n(14\,°C)=1.383\,82$.
(3) not specified.

Estimated Error:

accuracy of weighing 0.0001 g.

Components:

(1) Methanol (methyl alcohol);CH_4O; [67-56-1]
(2) Hexane (n-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. Suhrmann and R. Walter, Abh. Braunschw. Wiss. Ges. **3**, 135–52 (1951).

Variables:

T/K=311–323

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	vol% of H_2O	x_1	x_2	w_1	w_2
			(compiler)		(compiler)	
38.1	311.25	0.173	0.5299	0.4680	0.2961	0.7033
40.0	313.15	0.276	0.5293	0.4675	0.2960	0.7030
42.0	315.15	0.378	0.5286	0.4669	0.2958	0.7028
44.1	317.25	0.476	0.5280	0.4664	0.2957	0.7025
48.0	321.15	0.667	0.5268	0.4653	0.2955	0.7020
48.1	321.25	0.680	0.5267	0.4652	0.2955	0.7019
50.1	323.25	0.778	0.5261	0.4647	0.2954	0.7017

Auxiliary Information

Method/Apparatus/Procedure:

To the binary methanol–hexane mixture of constant composition (74.1 vol. % of hexane) known amounts of water were added and the turbidity temperature was measured. A linear relationship was obtained for change of turbidity temperature with number of moles of water in 1000 moles of methanol.

Source and Purity of Materials:

(1) Riedel de Haen and Merck, pure for analysis grade; dried over CaO for 2 weeks, distilled over $Mg(ClO_4)_2$; b.p. =64.78 °C, n(18 °C,D)=1.3292, d(16.3 °C,4 °C) =0.7950–0.7955.
(2) Ruhrchemie Holten; distilled three times; b.p.=68.8 °C, d(20 °C,4 °C)=0.6608.
(3) not specified.

Estimated Error:

temp. ±0.1 °C.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. B. Kogan, I. V. Deizenrot, T. A. Kulbyaeva, and V. M. Fridman, Zh. Prikl. Khim. (Leningrad) **29**, 1387–92 (1956).

Variables:

T/K=283–293

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/ °C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)		hydrocarbon-rich phase		hydrocarbon-poor phase	
10.0	283.15	0.1217	0.8783	0.8748	0.1252	0.049	0.951	0.722	0.278
		0.0342	0.9658	0.8236	0.0201	0.013	0.987	0.853	0.056
		0.0251	0.9749	0.7303	0.0067	0.0095	0.9905	0.815	0.020
		0.0064	0.9936	0.5840	0.0000	0.0024	0.9976	0.714	0.000
20.0	293.15	0.1811	0.8189	0.8157	0.1843	0.076	0.924	0.622	0.378
		0.0520	0.9480	0.8177	0.0278	0.020	0.980	0.835	0.0763
		0.0470	0.9530	0.7270	0.0080	0.018	0.982	0.810	0.024
		0.0316	0.9684	0.6480	0.0032	0.012	0.988	0.760	0.010
		0.0186	0.9814	0.5829	0.0006	0.007	0.993	0.712	0.002

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The two phase mixture was periodically shaken in a thermostated burette with water jacket for several hours. The phases were removed for analysis after separation. Methanol was determined by reaction with phthalic anhydride; water was determined by the Karl Fischer method. Water concentration in hydrocarbon-rich phase was smaller than 0.01–0.02%.

Source and Purity of Materials:

(1) source not specified, pure grade; distilled; contained <0.01% of water; n(20 °C)=1.3391.
(2) source not specified; used as received; b.p.=68.7 °C, n(20 °C)=1.3753.
(3) not specified.

Estimated Error:

temp. ±0.05 °C; soly.<±1% (relative error of methanol concentration).

Components:

(1) Methanol (methyl alcohol); CH^{4}O; [67-56-1]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **438-76**, 1–12 (1976).

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/ °C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
20	293.2	0.0000	0.99963	0.0000	0.000003	0.0000	0.99992	0.0000	0.000014
		0.0051	0.9944	0.1847	0.0000	0.0019	0.9980	0.2872	0.0001
		0.0099	0.9896	0.3497	0.0001	0.0037	0.9962	0.4887	0.0004
		0.0160	0.9835	0.5206	0.0008	0.0060	0.9939	0.6575	0.0027
		0.0246	0.9749	0.6428	0.0025	0.0093	0.9906	0.7572	0.0079
		0.0362	0.9629	0.7513	0.0091	0.0138	0.9860	0.8252	0.0269
		0.0444	0.9547	0.7958	0.0126	0.0170	0.9828	0.8489	0.0362
		0.0718	0.9268	0.8576	0.0336	0.0280	0.9717	0.8498	0.0895
		0.1394	0.8590	0.8822	0.0785	0.0569	0.9427	0.7909	0.1893
		0.2360	0.7640	0.8390	0.1610	0.1030	0.8970	0.6596	0.3404

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. The mole fraction of hydrocarbon in the charge before separation was about 0.30. After separation phases were analyzed by glc to determine methanol and hydrocarbon; concentration of water was determined by the Karl Fischer method.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified; distilled; purity >99.9%.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.03)

3.9. Methanol + Water + Toluene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of methanol between phases (distr.) for the system methanol–toluene–water is given in Table 10.

TABLE 10. Summary of experimental data for the system methanol–toluene–water

Author(s)	T/K	Type of data[a]	Ref.
Mason and Washburn, 1937	298	sol. (13), distr. (7)	1
Leikola, 1940	293	sol. (8)	2
Letcher and Siswana, 1992	298	sol. (14), Eq. (6)	3

[a] Number of experimental points in parentheses.

Saturation curve

The system methanol–toluene–water forms a miscibility gap of type 1. Only one binary system, toluene–water, is partially miscible. Data for this system were compiled and critically evaluated in a previously published SDS volume.[4] The recommended values of mutual solubility of toluene–water system at 298.2 K are: $x_2'=0.9972$ and $x_2''=0.000104$, by Ref. 4. This critical evaluation is based on the original papers with the exception of data of Leikola,[2] which were taken from the handbook of Kafarov;[5] this data set was also taken into account during evaluation but is not reported as a compilation sheet because it does not contribute further to knowledge of the system. The end points of saturation curve[3] were reported to be $x_2=0.999$ and pure water which is inconsistent with recommended values but within the accuracy of experimental measurements (0.001 mole fraction) stated by the authors. The experimental saturation data reported in Refs. 1 and 3 at 298.2 K show similar behavior of the system with differences in the most difficult to measure region, close to the plait point. In this region, $0.15<x_2<0.6$, Mason and Washburn[1] reported a slightly larger miscibility gap (about 0.04 mole fraction of water) than did Letcher and Siswana.[3] Leikola[2] at 293.2 K presents a smaller solubility gap than Ref. 1, but a little larger than Ref. 3. It seems, that results of Letcher and Siswana[3] at 298 K are the most reasonable. Therefore only data of Ref. 3 presenting saturation and equilibrium data were used to derive the equation:

$$x_1=1.0652+0.1260\ln(x_2)-1.1183x_2+0.0591x_2^2.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0070. The equation is valid in the region of $0.02<x_2<0.94$. Selected points on the saturation curve, calculated by this equation together with the ''best'' values of Ref. 4 are presented in Table 11 and as solid line in Fig. 5. The water-rich branch of saturation curve contains only a small amount of toluene ($x_2<0.0001$) and toluene was not detected in either study. These experimental points are not described by any model. The maximum methanol concentration observed on the saturation curve at 298 K was $x_1=0.68\pm0.01$.

TABLE 11. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x	x_2
0.0000	0.000 104 Ref. 4	0.4335	0.500
0.5499	0.020	0.4173	0.520
0.6150	0.040	0.4009	0.540
0.6438	0.060	0.3844	0.560
0.6579	0.080	0.3678	0.580
0.6638	0.100	0.3511	0.600
0.6647	0.120	0.3343	0.620
0.6621	0.140	0.3175	0.640
0.6569	0.160	0.3005	0.660
0.6498	0.180	0.2835	0.680
0.6411	0.200	0.2664	0.700
0.6313	0.220	0.2493	0.720
0.6204	0.240	0.2321	0.740
0.6087	0.260	0.2148	0.760
0.5963	0.280	0.1976	0.780
0.5833	0.300	0.1803	0.800
0.5698	0.320	0.1629	0.820
0.5559	0.340	0.1456	0.840
0.5415	0.360	0.1282	0.860
0.5269	0.380	0.1108	0.880
0.5119	0.400	0.0933	0.900
0.4966	0.420	0.0759	0.920
0.4811	0.440	0.0584	0.940
0.4654	0.460	0.0000	0.9972 Ref. 4
0.4496	0.480		

Phases in equilibrium

Compositions of coexisting phases in equilibrium of the ternary system methanol–toluene–water were reported only in Ref. 3. The tie lines are consistent with one another. They are considered tentative. Experimental tie lines together with all experimental saturation points at 298.2 K are presented in Fig. 5. The calculated plait point of the system at 293.2 K, Ref. 3, was $x_1 = 0.43$, $x_2 = 0.50$.

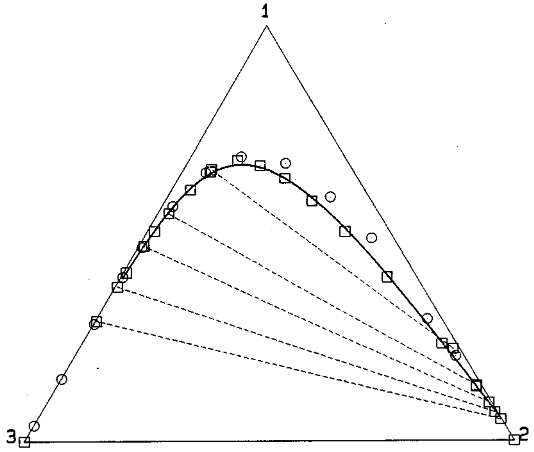

FIG. 5. Phase diagram of the system methanol (1)—toluene (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 1, □—experimental data, Ref. 3, dashed lines—experimental tie lines, Ref. 3.

References:

[1] L. S. Mason and E. R. Washburn, J. Am. Chem. Soc. **59**, 2076 (1937).

[2] E. Leikola, Suomen Kemistil. B **13**, 13 (1940).

[3] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

[4] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon New York, 1989).

[5] V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskva, 1963).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. S. Mason and E. R. Washburn, J. Am. Chem. Soc. **59**, 2076–7 (1937).

Variables:

$T/K = 298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

		x_1	x_2		
$t/$ °C	T/K (compiler)	(compiler)		w_1	w_2
25	298.2	0.2040	0.7785	0.0832	0.9128
		0.2937	0.6766	0.1302	0.8624
		0.4869	0.4675	0.2622	0.7240
		0.5867	0.3343	0.3684	0.6037
		0.6686	0.2021	0.5056	0.4394
		0.6841	0.1033	0.6215	0.2699
		0.6454	0.0491	0.6735	0.1472
		0.5648	0.0215	0.6573	0.0720
		0.4657	0.0077	0.5940	0.0283
		0.3948	0.0035	0.5312	0.0137
		0.2828	0.0012	0.4106	0.0050
		0.1510	0.0003	0.2400	0.0014
		0.0389	0.0001	0.0672	0.0006

Distribution of methanol in methanol–toluene–water system

		w_1'	w_1''
$t/$°C	T/K (compiler)	hydrocarbon-rich phase	water-rich phase
25	298.2	0.000	0.025
		0.001	0.101
		0.002	0.154
		0.002	0.220
		0.004	0.322
		0.008	0.406
		0.022	0.428

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Water was added to binary alcohol–toluene mixtures of known composition until the saturation point was reached. The refractive indexes of these mixtures were determined with an immersion refractometer and then were used to construct the refractive index/composition curve, which was used further to find compositions of equilibrium phases.

Source and Purity of Materials:

(1) synthetically prepared; dried over lime, distilled; $d(25\ °C, 4\ °C) = 0.78672$, $n(25\ °C, D) = 1.326\ 60$.
(2) Mallinckrodt, reagent grade; dried over Na, distilled; $d(25\ °C, 4\ °C) = 0.862\ 16$, $n(25\ °C, D) = 1.493\ 75$.
(3) distilled from $KMnO_4$.

Estimated Error:

Not reported.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

$T/K = 298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

				w_1	w_2
$t/$°C	T/K (compiler)	x_1	x_2	(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.405	0.006	0.538	0.023
		0.504	0.014	0.618	0.049
		0.604	0.038	0.660	0.119
		0.648	0.057	0.663	0.168
		0.675	0.100	0.620	0.264
		0.662	0.153	0.549	0.365
		0.632	0.219	0.470	0.468
		0.577	0.301	0.382	0.573
		0.502	0.406	0.292	0.678
		0.393	0.546	0.197	0.786
		0.234	0.736	0.099	0.894
		0.130	0.857	0.050	0.947
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/$°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.051	0.946	0.290	0.002	0.018	0.981	0.418	0.008
		0.068	0.926	0.372	0.004	0.025	0.974	0.507	0.016
		0.092	0.902	0.469	0.010	0.034	0.965	0.593	0.036
		0.133	0.856	0.547	0.022	0.051	0.946	0.642	0.074
		0.222	0.765	0.653	0.057	0.091	0.906	0.666	0.167

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; $d=0.786\,88$, $n=1.3265$.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) 1-Heptene; C_7H_{14}; [592-76-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, B. C. Bricknell, J. D. Sewry, and S. E. Radloff, J. Chem. Eng. Data **39**, 320–3 (1994).

Variables:

T/K=298

Compiled by:

A. Skrzecz

3.10. Methanol + Water + 1-Heptene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	1.000	0.000	1.000
		0.264	0.731	0.105	0.894
		0.454	0.539	0.215	0.783
		0.601	0.390	0.334	0.664
		0.707	0.283	0.448	0.549
		0.772	0.210	0.542	0.451
		0.805	0.165	0.606	0.381
		0.834	0.102	0.705	0.264
		0.827	0.053	0.782	0.154
		0.750	0.020	0.797	0.065
		0.554	0.012	0.664	0.044
		0.396	0.010	0.521	0.040
		0.239	0.006	0.351	0.027
		0.049	0.001	0.084	0.005
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.375	0.618	0.690	0.301	0.165	0.833	0.427	0.570
		0.240	0.754	0.805	0.165	0.094	0.905	0.606	0.381
		0.184	0.811	0.757	0.020	0.069	0.930	0.802	0.065
		0.116	0.881	0.571	0.017	0.041	0.958	0.668	0.061

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods have been described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) Aldrich; distilled; purity >99.8 mole % by glc., $\rho=0.692\,65$ g cm^{-3}.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.03)

3.11. Methanol + Water + Heptane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system methanol–heptane–water is given in Table 12.

TABLE 12. Summary of experimental data for the system methanol–heptane–water

Author(s)	T/K	Type of data[a]	Ref.
Bonner, 1909	273	sat. (7)	1
Kogan *et al.*, 1956	283, 293	Eq. (8)	2
Budantseva *et al.*, 1976	293, 313	Eq. (19)	3
Letcher *et al.*, 1986	298	sat. (8), Eq. (3)	4

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system methanol–heptane–water forms a very large miscibility gap of type 2 covering the majority of the concentration triangle. The system was studied at five temperatures in the range 273.2–298.2 K. Two binary systems, heptane–water and methanol–heptane form miscibility gap at the reported temperatures. Data for these binaries were compiled and critically evaluated in previously published SDS volumes, Refs. 5 and 6, respectively. In the binary methanol–heptane system the upper critical solution temperature is 324.3 ± 0.2 K.[6] This may be a reason for the large dispersion of solubility reported in the ternary system at temperatures over 300 K. Kogan *et al.*,[2] Budantseva *et al.*,[3] and Letcher *et al.*,[4] also report mutual solubility data for the binary methanol–heptane system; Refs. 3 and 4 report the same methanol concentration (0.176 mole fraction) at 293 and 298 K, respectively. Recommended solubilities of the binaries differ from those reported for the ternary system. The ternary data lack of one component in the phase. This is the result of very low concentrations (<0.001 mole fraction). The ternary solubilities reported in all data sets are consistent with one another. The data are considered tentative. The temperature 293.2 K was selected for presentation of the system behavior. The experimental saturation curve at 293.2 K is presented in Fig. 6. At this temperature the recommended values of mutual solubility are $x_2''=4.3\cdot 10^{-7}$, $x_3'=5.0\cdot 10^{-4}$, Ref. 5, for heptane–water system and $x_1''=0.1364$, $x_1'=0.9037$, Ref. 6, for methanol–heptane system. A fitting equation for the saturation curve was not derived because of the law quality of the experimental data. In a few studies the ternary compositions were reported as the binaries, the concentration of the third component was not detectable by the analytical method used. This situation was observed in hydrocarbon-rich phase as well as in hydrocarbon-poor phase.

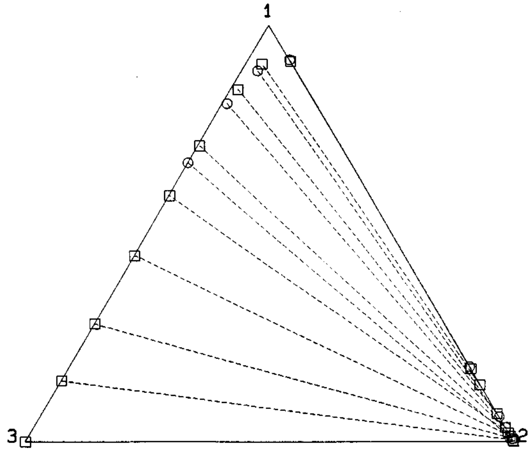

FIG. 6. Phase diagram of the system methanol (1)—heptane (2)—water (3) at 293.2 K. ○—experimental data, Ref. 2, □—experimental data, Ref. 3, dashed lines—experimental tie lines, Refs. 2 and 3.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system methanol–heptane–water were reported in the temperature range 283–313 K. The tie lines cover the whole area of miscibility gap. The reported equilibrium data sets are consistent with one another. All experimental points at 293.2 K, Refs. 2 and 3, are reported in Fig. 6.

References:

[1] W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).
[2] V. B. Kogan, I. V. Deizenrot, T. A. Kulbyaeva, and V. M. Fridman, Zh. Prikl. Khim. (Leningrad) **29**, 1387 (1956).
[3] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **437–76,** 1 (1976).
[4] T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn **18,** 1037 (1986).
[5] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).
[6] D. G. Shaw, A. Skrzecz, I. W. Lorimer, and A. Maczynski, eds., *Solubility Data Series*, Vol. 56, Alcohols with Hydrocarbons (Pergamon, New York, 1994).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910).

Variables:

$T/K=273$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
0.0	273.2	0.9283	0.0600	0.8270	0.1671
		0.9217	0.0434	0.8557	0.1261
		0.9109	0.0363	0.8641	0.1077
		0.9045	0.0263	0.8818	0.0803
		0.9010	0.0210	0.8915	0.0651
		0.8908	0.0155	0.8980	0.0490
		0.8610	0.0112	0.8895	0.0362
		0.8183	0.0077	0.8703	0.0257
		0.6321	0.0026	0.7475	0.0096

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diam and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogeneous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol–up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled; $n(14\ °C)=1.330\ 70$.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated Error:

accuracy of weighing 0.0001 g.

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Heptane (*n*-heptane);C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. B. Kogan, I. V. Deizenrot, T. A. Kulbyaeva, and V. M. Fridman, Zh. Prikl. Khim. (Leningrad) **29**, 1387–92 (1956).

Variables:

$T/K=283–293$

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

$t/°C$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)		hydrocarbon-rich phase		hydrocarbon-poor phase	
10.0	283.15	0.1099	0.8901	0.9217	0.0783	0.038	0.962	0.790	0.210
		0.0246	0.9754	0.8491	0.0177	0.008	0.992	0.867	0.0565
		0.0124	0.9876	0.7706	0.0053	0.004	0.996	0.844	0.018
		0.0093	0.9907	0.6988	0.0025	0.003	0.997	0.799	0.009
20.0	293.15	0.1810	0.8190	0.9159	0.0841	0.066	0.934	0.777	0.223
		0.0600	0.9400	0.8893	0.0322	0.020	0.980	0.860	0.0973
		0.0336	0.9664	0.8095	0.0096	0.011	0.989	0.860	0.032
		0.0065	0.9935	0.6672	0.0000	0.0021	0.9979	0.781	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The two phase mixture was periodically shaken in a thermostated burette with water jacket for several hours. The phases were removed for analysis after separation. Methanol was determined by reaction with phthalic anhydride; water was determined by the Karl Fischer method. Water concentration in hydrocarbon-rich phase was smaller than 0.01–0.02%.

Source and Purity of Materials:

(1) source not specified, pure grade; distilled; contained <0.01% of water; $n(20\ °C)=1.3391$.
(2) source not specified; used as received; b.p. = 98.4 °C, $n(20\ °C)=1.3877$.
(3) not specified.

Estimated Error:

temp. ±0.05 °C; soly. <±1% (relative error of methanol concentration).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **437–76**, 1–13 (1976).

Variables:

T/K = 293–313

Compiled By:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
20	293.2	0.0000	0.9995	0.0000	0.000 003	0.0000	0.999 91	0.0000	0.000 02
		0.0031	0.9964	0.1473	0.000 02	0.0010	0.9989	0.2350	0.000 10
		0.0072	0.9922	0.2841	0.0001	0.0023	0.9976	0.4136	0.0005
		0.0133	0.9861	0.4468	0.0002	0.0043	0.9956	0.5892	0.0008
		0.0215	0.9779	0.5895	0.0009	0.0070	0.9929	0.7166	0.0034
		0.0336	0.9658	0.7075	0.0040	0.0110	0.9889	0.8020	0.0142
		0.0676	0.9314	0.8431	0.0154	0.0227	0.9771	0.8684	0.0496
		0.1373	0.8612	0.9053	0.0334	0.0485	0.9512	0.8670	0.1000
		0.1760	0.8240	0.9120	0.0880	0.0639	0.9361	0.7682	0.2318
40	313.2	0.0000	0.9993	0.0000	0.000 01	0.0000	0.999 87	0.0000	0.000 06
		0.0041	0.9950	0.1508	0.000 02	0.0013	0.9985	0.2400	0.000 10
		0.0100	0.9889	0.3119	0.0001	0.0032	0.9966	0.4462	0.0004
		0.0168	0.9819	0.4608	0.0004	0.0054	0.9943	0.6024	0.0016
		0.0281	0.9704	0.5902	0.0017	0.0092	0.9906	0.7154	0.0064
		0.0467	0.9516	0.7382	0.0078	0.0154	0.9842	0.8153	0.0269
		0.0945	0.9036	0.8502	0.0214	0.0323	0.9673	0.8594	0.0676
		0.1400	0.8578	0.8971	0.0416	0.0496	0.9500	0.8450	0.1225
		0.2250	0.7725	0.8845	0.1005	0.0852	0.9143	0.7327	0.2603
		0.2950	0.7050	0.8350	0.1650	0.1180	0.8820	0.6181	0.3819

Auxiliary Information

Method/Apparatus/Procedure:

The method was described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **49**, 1849 (1975).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:

T/K = 298

Compiled by:

A. Skrzecz

Experimental Data

Compositions of the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.040	0.000	0.069	0.000
		0.144	0.000	0.230	0.000
		0.339	0.001	0.475	0.004
		0.580	0.002	0.706	0.008
		0.848	0.026	0.848	0.081
		0.880	0.038	0.842	0.114
		0.893	0.099	0.740	0.256
		0.176	0.824	0.064	0.936

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
25	298.2	0.115	0.885	0.886	0.042	0.040	0.960	0.838	0.124
		0.060	0.940	0.695	0.005	0.020	0.980	0.790	0.018
		0.003	0.997	0.400	0.000	0.001	0.999	0.542	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) Merck, Uvasol grade; dried with magnesium metal activated with iodine, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1] S. W. Briggs and E. W. Commings, Ind. Eng. Chem. **35**, 411 (1943).

Components:	**Evaluated by:**
(1) Methanol (methyl alcohol); CH_4O; [67-56-1] (2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.03)

3.12. Methanol + Water + *p*-Xylene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) for the system methanol–*p*-xylene–water is given in Table 13.

TABLE 13. Summary of experimental data for the system methanol–*p*-xylene–water

Author(s)	T/K	Type of data[a]	Ref.
Leikola, 1940	294	sat. (4)	1
Letcher, *et al.*, 1989	298	sat. (17), Eq. (5)	2

[a]Number of experimental points in parentheses.

Saturation curve

The system methanol–*p*-xylene–water forms a miscibility gap of type 1. Only one binary system, *p*-xylene–water, is partially miscible. The data for this system were compiled and critically evaluated in a previously published SDS volumes, Ref. 3. The recommended values of mutual solubility of *p*-xylene–water system at 298.2 K are: $x_2'=0.9974$ and $x_2''=0.000\ 031$. The data of Leikola[1] taken from the handbook of Kafarov,[4] were also taken into account during evaluation but are not reported as compilation sheet because they do not contribute further to knowledge of the system. All experimental saturation data are consistent. The data of Letcher *et al.*[2] describe the whole binodal curve. The end points of saturation curve, Ref. 2, were reported to be $x_2=0.998$ and pure water which is inconsistent with recommended values. Data for the water-rich phase in the range of low methanol concentrations, Ref. 2, were reported to be *p*-xylene free. All these results are within the accuracy of experimental measurements which were stated by the authors to be 0.005 mole fraction. Phase equilibrium data, Ref. 2, were also used to construct the saturation curve with the exception of one point ($x_1=0.058$ $x_2=0.916$) which appears to contain experimental error. Data at 298.2 K, Ref. 2, presenting both phases (organic-rich and water-rich) were fitted by the equation:

$$x_1=1.1424+0.1264\ln(x_2)-1.2561x_2+0.1108x_2^2.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0194. The points on the saturation curve calculated by this equation for the selected concentrations of *p*-xylene together with the ''best'' values of Ref. 3 are presented in Table 14.

TABLE 14. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 031 Ref. 3	0.4365	0.5200
0.6228	0.0200	0.4185	0.5400
0.6855	0.0400	0.4004	0.5600
0.7118	0.0600	0.3823	0.5800
0.7234	0.0800	0.3641	0.6000
0.7269	0.1000	0.3458	0.6200
0.7253	0.1200	0.3275	0.6400
0.7202	0.1400	0.3091	0.6600
0.7126	0.1600	0.2907	0.6800
0.7031	0.1800	0.2723	0.7000
0.6922	0.2000	0.2539	0.7200
0.6800	0.2200	0.2355	0.7400
0.6669	0.2400	0.2171	0.7600
0.6530	0.2600	0.1986	0.7800
0.6385	0.2800	0.1802	0.8000
0.6234	0.3000	0.1618	0.8200
0.6078	0.3200	0.1434	0.8400
0.5918	0.3400	0.1250	0.8600
0.5754	0.3600	0.1067	0.8800
0.5588	0.3800	0.0883	0.9000
0.5419	0.4000	0.0700	0.9200
0.5247	0.4200	0.0517	0.9400
0.5074	0.4400	0.0335	0.9600
0.4899	0.4600	0.0153	0.9800
0.4722	0.4800	0.0000	0.9974 Ref. 3
0.4544	0.5000		

Phases in equilibrium

Compositions of coexisting phases in equilibrium of the ternary system methanol–*p*-xylene–water were reported only by Letcher *et al.*[2] The tie lines are consistent with one another and cover the whole area of the miscibility gap. One point for organic-rich phase ($x_1=0.058$, $x_2=0.916$) appears to contain any experimental error. The phase equilibrium data are considered tentative. All experimental saturation points together with experimental tie lines at 298.2 K are presented in Fig. 7. The plait point of the system at 298.2 K, calculated by Letcher and Siswana[5] was reported to be $x_1=0.46$, $x_2=0.49$.

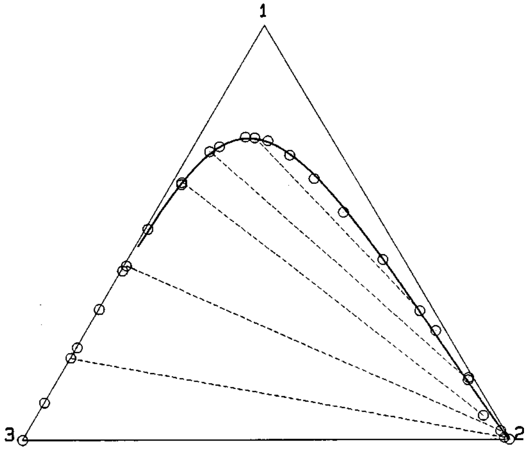

FIG. 7. Phase diagram of the system methanol (1)—*p*-xylene (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 2, dashed lines—experimental tie lines, Ref. 2.

References:

[1]E. Leikola, Suomen. Kemistil. B **13**, 13 (1940).

[2]T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

[3]D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons, C_8 to C_{36} (Pergamon, New York, 1989).

[4]V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentny e Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskva, 1963).

[5]T. M. Letcher, and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:
(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053–60 (1989).

Variables:
T/K=298

Compiled by:
A. Skrzecz

Experimental Data

Compositions of the saturation curve

t/°C	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.998	0.000	0.9997
		0.150	0.840	0.051	0.947
		0.263	0.716	0.099	0.896
		0.433	0.523	0.198	0.791
		0.548	0.385	0.294	0.685
		0.629	0.285	0.388	0.582
		0.686	0.207	0.479	0.479
		0.721	0.145	0.565	0.376
		0.730	0.095	0.639	0.275
		0.707	0.053	0.695	0.173
		0.615	0.021	0.692	0.078
		0.508	0.005	0.636	0.021
		0.407	0.003	0.544	0.013
		0.315	0.001	0.448	0.005
		0.224	0.001	0.338	0.005
		0.090	0.000	0.150	0.000
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C (compiler)	T/K	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.310	0.660	0.728	0.115	0.123	0.870	0.608	0.318
		0.144	0.842	0.695	0.039	0.049	0.948	0.714	0.133
		0.058	0.916	0.620	0.019	0.019	0.977	0.700	0.071
		0.021	0.970	0.419	0.005	0.006	0.992	0.552	0.022
		0.005	0.985	0.199	0.000	0.002	0.997	0.306	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. A binary mixture of known composition was titrated with the third component until cloudiness was observed. Tie line compositions were related to the coexistence curve; water was determined by the Karl Fischer titration. The methods were described in Ref. 1.

Source and Purity of Materials:
(1) source not specified; used as received.
(2) source not specified; recrystallized three times.
(3) not specified.

Estimated Error:
comp. <0.005 mole fraction (estimated authors' precision on binodal curve), <0.01 mole fraction (estimated authors' precision of tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

Components:	**Original Measurements:**
(1) Methanol (methyl alcohol); CH_4O; [67-56-1] (2) Xylene (mixture of isomers); C_8H_{10}; [1330-20-7] (3) Water; H_2O; [7732-18-5]	J. Hartley, J. Soc. Chem. Ind. (London) **69**, 60–1 (1950).
Variables: T/K=293–323	**Compiled by:** A. Skrzecz

3.13. Methanol + Water + Xylene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
20	293.2	0.419	0.553	0.185	0.808
		0.696	0.229	0.465	0.507
		0.765	0.092	0.666	0.264
		0.758	0.062	0.711	0.194
		0.725	0.039	0.735	0.130
		0.696	0.029	0.736	0.100
		0.611	0.013	0.706	0.050
		0.356	0.002	0.492	0.010
30	303.2	0.416	0.548	0.185	0.806
		0.686	0.226	0.462	0.505
		0.749	0.089	0.660	0.260
		0.742	0.061	0.703	0.192
		0.701	0.038	0.721	0.128
		0.680	0.028	0.726	0.099
		0.611	0.014	0.703	0.054
		0.356	0.003	0.491	0.012
50	323.2	0.243	0.719	0.092	0.900
		0.412	0.544	0.184	0.805
		0.708	0.155	0.545	0.396
		0.721	0.102	0.622	0.292
		0.710	0.065	0.675	0.205
		0.671	0.035	0.705	0.121
		0.545	0.009	0.660	0.036
		0.417	0.002	0.556	0.009

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20	293.2	0.101	0.888	0.636	0.015	0.033	0.965	0.721	0.057
30	303.2	0.106	0.883	0.638	0.018	0.035	0.963	0.715	0.068
50	323.2	0.146	0.833	0.637	0.024	0.050	0.946	0.702	0.088

Concentration of xylene and water in coexisting phases

		w'_2	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase	water-rich phase
20	293.2	0.983	0.517
		0.982	0.353
		0.977	0.254
		0.965	0.222
30	303.2	0.985	0.525
		0.977	0.351
		0.970	0.256
		0.963	0.217

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Binary mixtures of known volumes were titrated with the third component in glass-stoppered bottles until, after vigorously shaking, the mixture became turbid. The equilibrium phases were determined by titrating with water binary methanol–xylene mixtures. The xylene-rich phase was at the beginning the lower layer, but addition of water caused this phase to separate as the upper layer. To determine tie lines, mixtures of known composition were immersed in a thermostat bath, shaken, and after separation one component of each phase was analyzed. Water, in the alcohol-rich phase, was analyzed by the Karl Fischer reagent and xylene, in the hydrocarbon-rich phase, was determined by extraction with water. The results were presented on a Gibbs triangle together with binodal curve.

Source and Purity of Materials:

(1) BDH, sulphur free; distilled; fraction boiling at the range 140–2 °C was used.
(2) source not specified; absolute alcohol; used as received.
(3) distilled.

Estimated Error:

temp. ±0.5 °C (temperature of the bath).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.05)

3.14. Methanol + Water +2,2,4-Trimethylpentane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system methanol–2,2,4-trimethylpentane–water is given in Table 15.

TABLE 15. Summary of experimental data for the system methanol–2,2,4-trimethylpentane–water

Author(s)	T/K	Type of data[a]	Ref.
Buchowski and Teperek, 1959	291, 293	sat. (21), eq. (18)	1
Budantseva *et al.*, 1976	293	eq. (6)	2

[a] Number of experimental points in parentheses.

Saturation curve

The system methanol–2,2,4-trimethylpentane–water forms a large miscibility gap of type 2 covering the majority of the concentration triangle. Two binary systems 2,2,4-trimethylpentane–water and 2,2,4-trimethylpentane–methanol are partially miscible. The data for these systems were compiled and critically evaluated in previously, published SDS volumes, Refs. 3 and 4. The recommended values of mutual solubility of 2,2,4-trimethylpentane–water system, Ref. 3, and methanol–2,2,4-trimethylpentane system, Ref. 4, at 293 K are: $x_2'=0.9995$, $x_2''=3\cdot10^{-7}$ and $x_2'=0.890$, $x_2''=0.224$, respectively. (The mutual solubilities of methanol–2,2,4-trimethylpentane system, reported in both papers[1,2] were also considered during evaluation of this binary system in Ref. 4.) Compositions along the saturation curve at 291.2 and 293.2 K by Buchowski and Teperek[1] were obtained by the titration method. They are consistent within each data set, as well as with one another. The paper of Budantseva *et al.*[2] contains information about phases in equilibrium at 293.2 K only. The hydrocarbon-poor phase shows smaller miscibility while the hydrocarbon-rich phase shows larger solubility[2] than data of Ref. 1 at the same temperature and than the ''best'' binary solubilities by Ref. 4. The data of Buchowski and Teperek[1] were well documented (description of the method, description of pure substances properties and purity) while data of Ref. 2 were reported without any auxiliary information. Therefore data of Ref. 1 appear reliable, but all are considered as tentative.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system methanol–2,2,4-trimethylpentane–water were reported in both references. Tie lines cover nearly the whole range of miscibility gap. In the paper of Buchowski and Teperek[1] the reported hydrocarbon-rich phase did not contain detectable water (water concentration in the hydrocarbon-rich phase was neglected because solubility of water in 2,2,4-trimethylpentane is lower than 0.000 5 mass fraction, Ref. 1). The data from Refs. 1 and 2 show slightly different directions of the tie lines. All of them are considered as tentative. To present system behavior, experimental data along the saturation curve and experimental compositions of coexisting phases in equilibrium at 293.2 K, are presented in Fig. 8.

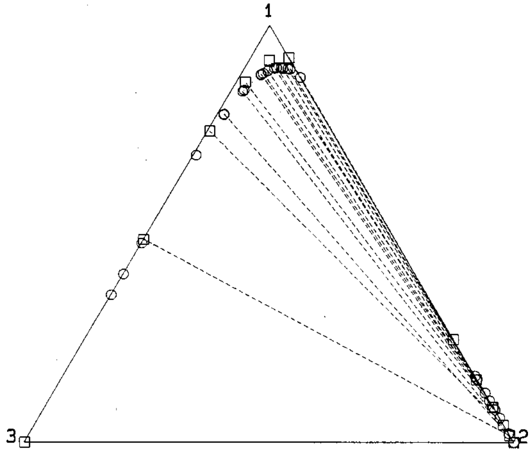

FIG. 8. Phase diagram of the system methanol (1)—2,2,4-trimethylpentane (2)—water (3) at 293.2 K. ○—experimental data, Ref. 1, □—experimental data, Ref. 2, dashed lines—experimental tie lines, Refs. 1 and 2.

References:

[1] H. Buchowski and J. Teperek, Rocz. Chem. **33**, 1093 (1959).
[2] L. S. Budantseva, T.M. Lesteva, and M.S. Nemtsov, Dep. Doc. VINITI **437–76,** 1 (1976).
[3] D.G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).
[4] D. G. Shaw, A. Skrzecz, J. W. Lorimer, and A. Maczynski, eds., *Solubility Data Series*, Vol. 56, Alcohols with Hydrocarbons (Pergamon, New York, 1994).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

H. Buchowski and J. Teperek, Rocz. Chem. **33**, 1093–8 (1959).

Variables:

$T/K = 291-293$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
18	291.2	0.8786	0.1214	0.670	0.330
		0.9071	0.0780	0.760	0.233
		0.9054	0.0639	0.787	0.198
		0.9002	0.0558	0.801	0.177
		0.8940	0.0442	0.823	0.145
		0.8880	0.0350	0.841	0.118
		0.8359	0.0200	0.846	0.072
		0.7192	0.0073	0.800	0.029
		0.6227	0.0007	0.744	0.003
		0.3985	0.0004	0.540	0.002
		0.3076	0.0002	0.441	0.001
20	293.2	0.8747	0.1253	0.662	0.338
		0.8988	0.0740	0.763	0.224
		0.8970	0.0606	0.789	0.190
		0.8811	0.0408	0.823	0.136
		0.8441	0.0251	0.838	0.089
		0.7845	0.0135	0.829	0.051
		0.6875	0.0057	0.781	0.023
		0.4769	0.0007	0.617	0.003
		0.4033	0.0004	0.545	0.002
		0.3538	0.0002	0.493	0.001

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/°C$	T/K (compiler)	hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)		hydrocarbon-rich phase		hydrocarbon-poor phase	
18	291.2	0.1773	0.8227	0.8786	0.1214	0.057	0.943	0.670	0.330
		0.1054	0.8946	0.9025	0.0705	0.032	0.968	0.772	0.215
		0.1524	0.8476	0.9055	0.0775	0.048	0.952	0.760	0.232
		0.0869	0.9131	0.9045	0.0519	0.026	0.974	0.812	0.166
		0.0806	0.9194	0.8971	0.0415	0.024	0.976	0.831	0.137
		0.0678	0.9322	0.8866	0.0346	0.020	0.980	0.841	0.117
		0.0448	0.9552	0.8535	0.0231	0.013	0.987	0.849	0.082
		0.0415	0.9585	0.8363	0.0197	0.012	0.988	0.847	0.071
		0.0000	1.0000	0.7200	0.0060	0.000	1.000	0.804	0.024
20	293.2	0.1580	0.8420	0.8950	0.0940	0.050	0.950	0.724	0.271
		0.1495	0.8505	0.8957	0.0891	0.047	0.953	0.733	0.260
		0.1175	0.8825	0.8961	0.0784	0.036	0.964	0.753	0.235
		0.0993	0.9007	0.8983	0.0649	0.030	0.970	0.781	0.201
		0.0838	0.9162	0.8910	0.0501	0.025	0.975	0.808	0.162
		0.0774	0.9226	0.8848	0.0440	0.023	0.977	0.818	0.145
		0.0581	0.9419	0.8821	0.0415	0.017	0.983	0.822	0.138
		0.0211	0.9789	0.8411	0.0236	0.006	0.994	0.840	0.084
		0.0000	1.0000	0.7860	0.0135	0.000	1.000	0.830	0.051

Auxiliary Information

Method/Apparatus/Procedure:

Solubility was measured by the titration method. Known masses of methanol and water were titrated with 2,2,4-trimethylpentane until turbidity was observed. The mass of hydrocarbon was determinated from mass balance of the mixture. To obtain equilibrium data, known masses of components were shaken and allowed to stand for over 2 h. Refractive indexes of the hydrocarbon-rich phase were measured and phase composition was read from the calibration curve of the binary methanol–2,2,4-trimethylpentane mixture. Water concentration in the hydrocarbon-rich phase was neglected because the solubility of water in 2,2,4-trimethylpentane is lower than 0.000 05 mass fraction.[1] Concentration of the water-rich phase was determined graphically from a large scale ternary diagram from the binodal curve, composition of hydrocarbon-rich phase and total composition of starting mixture.

Source and Purity of Materials:

(1) F. O. Ch. Gliwice, pure grade; boiled with I_2 and Mg to remove water, distilled; middle fraction was used; $n(20\ °C) = 1.3288$, $\rho(20\ °C) = 0.7915\ g/c^3$.
(2) obtained from the Physical Chemistry Department of Warsaw University, high purity grade; distilled only to remove water; $n(20\ °C) = 1.3914$, $\rho(20\ °C) = 0.6920\ g/cm^3$.
(3) doubly distilled.

Estimated Error:

temp. ±0.5 °C.

References:

[1] A. Weissberger, E. S. Proskauer, I. A. Riddick, and E. E. Toops, *Organic Solvents*, 2nd ed. (New York, 1995).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **437–76**, 1–13 (1976).

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
20	293.2	0.0000	0.999 56	0.0000	0.000 000 3	0.0000	0.999 931	0.0000	0.000 002
		0.0162	0.9831	0.4855	0.0002	0.0046	0.9953	0.6262	0.0009
		0.0414	0.9579	0.7456	0.0043	0.0120	0.9879	0.8270	0.0170
		0.0836	0.9152	0.8636	0.0180	0.0250	0.9748	0.8685	0.0645
		0.1493	0.8490	0.9158	0.0411	0.0470	0.9527	0.8428	0.1349
		0.2460	0.7540	0.9220	0.0780	0.0838	0.9162	0.7683	0.2317

Auxiliary Information

Method/Apparatus/Procedure:

The method was described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **49**, 1849 (1975).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Octane (*n*-octane); C_8H_{18}; [111-65-9]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.04)

3.15. Methanol + Water + Octane

Critical Evaluation:

A survey of reported compositions along the saturation curve and compositions of coexisting phases in equilibrium (eq.) for the system methanol–octane–water is given in Table 16.

TABLE 16. Summary of experimental data for the system methanol–octane–water

Author(s)	T/K	Type of data[a]	Ref.
Kogan *et al.*, 1956	283, 293	eq. (12)	1
Budantseva *et al.*, 1976	293	eq. (10)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system methanol–octane–water forms a large miscibility gap of type 2 covering the majority of the concentration triangle. Compositions along the saturation curves were not reported independently in the references; the saturation curves can be constructed on the bases of equilibrium compositions. Two binary systems, octane–water and octane–methanol, form miscibility gaps. The data for these systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. The recommended, Ref. 3, values of mutual solubility of octane–water system at 293 K[4] are: $x''_2=9.9\cdot 10^{-8}$ and $x'_2=0.9995$. The mutual solubility of methanol–octane system at 293 K,[4] are: $x''_1=0.944$ and $x'_1=0.105$. The binary data reported by Budantseva *et al.*[2] are: $x''_2=2.0\cdot 10^{-7}$, $x'_2=0.999\,57$ and $x''_1=0.960$, $x'_1=0.155$, respectively.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system methanol–octane–water were reported in both references. The experimental procedure was reported only in Ref. 1. After separation, methanol was determined by reaction with phthalic anhydride; water—with the Karl Fischer reagent. The compositions of phases in equilibrium reported in Refs. 1 and 2 are consistent with one another, they are treated as tentative and those at 293.2 K are presented in Fig. 9.

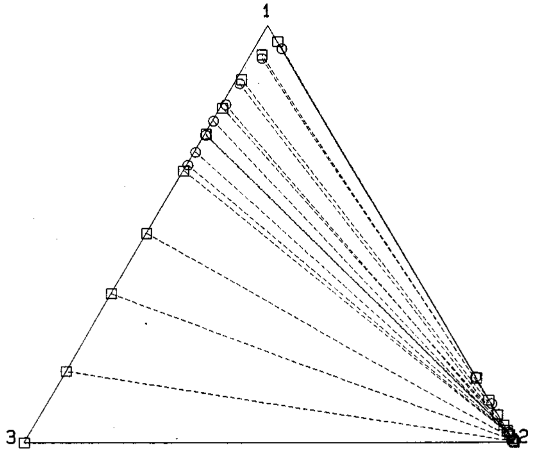

FIG. 9. Phase diagram of the system methanol (1)—octane (2)—water (3) at 293.2 K. ○—experimental data, Ref. 1, □—experimental data, Ref. 2, dashed lines—experimental tie lines, Ref. 2.

References:

[1] V. B. Kogan, I. V. Deizenrot, T. A. Kulbyaeva, and V. M. Fridman, Zh. Prikl. Khim. (Leningrad) **29**, 1387 (1956).

[2] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Dep. Doc. VINITI **437–76,** 1 (1976).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

[4] D. G. Shaw, A. Skrzecz, W. Lorimer, and A. Maczynski, eds., *Solubility Data Series*, Vol. 56, Alcohols with Hydrocarbons (Pergamon, New York, 1994).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Octane (*n*-octane); C_8H_{18}; [111-65-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. B. Kogan, I. V. Deizenrot, T. A. Kulbyaeva, and V. M. Fridman, Zh. Prikl. Khim. (Leningrad) **29**, 1387–92 (1956).

Variables:

T/K = 283–293

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)		hydrocarbon-rich phase		hydrocarbon-poor phase	
10.0	283.15	0.0742	0.9258	0.9507	0.0493	0.022	0.978	0.844	0.156
		0.0482	0.9518	0.9107	0.0211	0.014	0.986	0.889	0.0736
		0.0245	0.9755	0.8106	0.0063	0.007	0.993	0.866	0.024
		0.0245	0.9755	0.6856	0.0000	0.007	0.993	0.795	0.000
20.0	293.15	0.1580	0.8420	0.9431	0.0569	0.050	0.950	0.823	0.177
		0.0931	0.9069	0.9197	0.0275	0.028	0.972	0.878	0.0937
		0.0242	0.9758	0.8602	0.0114	0.0069	0.9931	0.8840	0.0418
		0.0141	0.9859	0.8098	0.0079	0.004	0.996	0.861	0.030
		0.0141	0.9859	0.7708	0.0020	0.004	0.996	0.851	0.008
		0.0211	0.9789	0.7368	0.0028	0.006	0.994	0.825	0.011
		0.0176	0.9824	0.6955	0.0027	0.005	0.995	0.795	0.011
		0.0176	0.9824	0.6645	0.0022	0.005	0.995	0.773	0.009

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The two phase mixture was periodically shaken in a thermostated burette with water jacket for several hours. The phases were removed for analysis after separation. Methanol was determined by reaction with phthalic anhydride; water was determined by the Karl Fischer method. Water concentration in the hydrocarbon-rich phase was smaller than 0.01–0.02%.

Source and Purity of Materials:

(1) source not specified, pure grade; distilled; contained <0.01% of water; $n(20\ °C) = 1.3391$.
(2) source not specified; used as received; b.p. = 125.4°C, $n(20\ °C) = 1.3976$.
(3) not specified.

Estimated Error:

temp. ±0.05 °C; soly. <±1% (relative error of methanol concentration).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Octane (*n*-octane); C_8H_{18}; [111-65-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. S. Budantseva, T. M. Lesteva and M. S. Nemtsov, Dep. Doc. VINITI **437–76**, 1–13 (1976).

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
20	293.2	0.0000	0.99957	0.0000	0.000 000 2	0.0000	0.999 932	0.0000	0.000 001
		0.0018	0.9975	0.1722	0.000 02	0.0005	0.9994	0.2700	0.000 11
		0.0050	0.9943	0.3554	0.0001	0.0014	0.9985	0.4949	0.0005
		0.0092	0.9901	0.4995	0.0002	0.0026	0.9973	0.6392	0.0009
		0.0182	0.9811	0.6501	0.0009	0.0052	0.9947	0.7652	0.0038
		0.0279	0.9714	0.7390	0.0027	0.0080	0.9919	0.8268	0.0108
		0.0414	0.9579	0.8016	0.0052	0.0120	0.9879	0.8631	0.0200
		0.0671	0.9322	0.8694	0.0109	0.0198	0.9801	0.8912	0.0398
		0.1022	0.8966	0.9283	0.0233	0.0310	0.9688	0.8938	0.0800
		0.1550	0.8450	0.9600	0.0400	0.0489	0.9511	0.8707	0.1293

Auxiliary Information

Method/Apparatus/Procedure:

The method was described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **49**, 1849 (1975).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12}; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T.M. Letcher and P.M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled By:

A. Skrzecz

3.16. Methanol + Water + Mesitylene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.360	0.001	0.498	0.005
		0.457	0.002	0.595	0.010
		0.565	0.005	0.684	0.023
		0.734	0.022	0.770	0.087
		0.788	0.043	0.755	0.154
		0.796	0.053	0.737	0.184
		0.807	0.092	0.668	0.285
		0.792	0.141	0.583	0.389
		0.747	0.202	0.487	0.494
		0.682	0.273	0.394	0.591
		0.595	0.370	0.297	0.693
		0.471	0.503	0.199	0.795
		0.292	0.690	0.101	0.895
		0.163	0.826	0.050	0.948
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		hydrocarbon-poor phase		hydrocarbon-rich phase (compiler)		hydrocarbon-poor phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.090	0.905	0.533	0.001	0.026	0.973	0.667	0.005
		0.140	0.852	0.663	0.010	0.042	0.957	0.750	0.042
		0.200	0.790	0.755	0.023	0.063	0.935	0.781	0.089
		0.208	0.717	0.800	0.056	0.071	0.915	0.733	0.193
		0.408	0.573	0.795	0.135	0.159	0.837	0.593	0.378

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; $d = 0.786\,88$, $n = 1.3265$.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wooten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) Nonane (*n*-nonane); C_9H_{20}; [111-84-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. B. Kogan, I. V. Deizenrot, T. A. Kulbyaeva, and V. M. Fridman, Zh. Prikl. Khim. (Leningrad) **29**, 1387–92 (1956).

Variables:

$T/\text{K} = 283-293$

Compiled by:

A. Skrzecz

3.17. Methanol + Water + Nonane

Experimental Data

Compositions of coexisting phases

$t/°\text{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-lean phase (compiler)		hydrocarbon-rich phase (compiler)		hydrocarbon-lean phase		hydrocarbon-rich phase	
10.0	283.15	0.9615	0.0385	0.0965	0.9035	0.862	0.138	0.026	0.974
		0.9458	0.0183	0.0501	0.9499	0.910	0.0706	0.013	0.987
		0.8957	0.0081	0.0464	0.9536	0.912	0.0329	0.012	0.988
		0.7512	0.0000	0.0236	0.9764	0.843	0.000	0.006	0.994
20.0	293.15	0.9562	0.0438	0.1034	0.8966	0.845	0.155	0.028	0.972
		0.9370	0.0220	0.0861	0.9139	0.894	0.0840	0.023	0.977
		0.9238	0.0138	0.0381	0.9619	0.911	0.0544	0.0098	0.9902
		0.7725	0.0009	0.0158	0.9842	0.855	0.004	0.0040	0.9960

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The two phase mixture was periodically shaken in a thermostated burette with water jacket for several hours. The phases were removed for analysis after separation. Methanol was determined by reaction with phthalic anhydride; water was determined by the Karl Fischer method. Water concentration in the hydrocarbon-rich phase was smaller than 0.01–0.02%.

Source and Purity of Materials:

(1) source not specified, pure grade; distilled; contained <0.01% of water; $n(20\ °\text{C}) = 1.3391$.
(2) source not specified; used as received; b.p. $= 150.5\ °\text{C}$, $n(25\ °\text{C}) = 1.4035$.
(3) not specified.

Estimated Error:

temp. $\pm 0.05\ °\text{C}$; soly. $< \pm 1\%$ (relative error of methanol concentration).

Components:

(1) Methanol (methyl alcohol); CH_4O; [67-56-1]
(2) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements

C. F. Prutton, T. J. Walsh, and A. M. Desai, Ind. Eng. Chem. **42**, 1210–7 (1950).

Variables:

T/K=298 and 308

Compiled by:

A. Skrzecz

3.18. Methanol + Water + 1-Methylnaphthalene

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon -rich phase		water -rich phase	
25.0	298.15	0.0000	1.0000	0.0000	0.0000	0.000	1.000	0.000	0.000
		0.0429	0.9571	0.2726	0.0000	0.010	0.990	0.400	0.000
		0.0511	0.9489	0.3957	0.0000	0.012	0.988	0.538	0.000
		0.0752	0.9248	0.6273	0.0058	0.018	0.982	0.730	0.030
		0.1022	0.8978	0.6928	0.0134	0.025	0.975	0.755	0.065
		0.1207	0.8793	0.7356	0.0242	0.030	0.970	0.752	0.110
		—	—	0.8023	0.0487	—	—	0.728	0.196
		—	—	0.8173	0.0555	—	—	0.720	0.217
		—	—	0.7973	0.1196	—	—	0.580	0.386
		—	—	0.7910	0.1507	—	—	0.530	0.448
35.0	308.15	0.0000	1.0000	0.0000	0.0000	0.000	1.000	0.000	0.000
		0.0511	0.9489	0.3957	0.0000	0.012	0.988	0.538	0.000
		0.0752	0.9248	0.6229	0.0078	0.018	0.982	0.720	0.040
		0.1022	0.8978	0.6885	0.0156	0.025	0.975	0.745	0.075
		—	—	0.7118	0.0188	—	—	0.752	0.088
		—	—	0.7741	0.0389	—	—	0.736	0.164
		—	—	0.7948	0.0552	—	—	0.707	0.218
		—	—	0.7993	0.0824	—	—	0.649	0.297
		—	—	0.7934	0.1189	—	—	0.579	0.385
		—	—	0.7390	0.1915	—	—	0.454	0.522
		—	—	0.6184	0.3223	—	—	0.297	0.687
		—	—	0.5184	0.4457	—	—	0.206	0.786
		—	—	0.4506	0.5494	—	—	0.156	0.844
		0.2021	0.7979	—	—	0.054	0.946	—	—
		0.3376	0.6624	—	—	0.103	0.897	—	—

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Samples in 4 oz. oil sample bottles were agitated in a constant temperature bath for at least 12 h before phase separation. Samples of each phase were taken for analysis by a rubber bulb pipette. Water was determined by the Karl Fischer reagent, hydrocarbons as the caustic-insoluble fraction, methanol–by the difference.

Source and Purity of Materials:

(1) Barker C.P. analyzed absolute; purity 99.5%; water-free by the Karl Fischer.
(2) (a) Eastman Kodak Co.; distillation range 238–240 °C, contained about 5% of 2-methylnaphtalene isomer. (b) prepared in the laboratory from the crude material; extracted with NaOH aq., refluxed with Na, distilled; fraction boiling at 240 °C was collected; contained about 10% of 2-methylnaphtalene isomer.
(3) not specified.

Estimated Error:

temp. ± 0.01 °C.

4. Ethanol+Water

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.05)

4.1. Ethanol + Water + Benzene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of ethanol between phases (distr.) for the system ethanol–benzene–water is given in Table 17.

TABLE 17. Summary of experimental data for the system ethanol–benzene–water

Author(s)	T/K	Type of data[a]	Ref.
Taylor, 1896	298	sat. (14), eq. (6)	1
Lincoln, 1899	298	sat. (13)	2
Bonner, 1909	288	sat. (12)	3
Holmes, 1918	288	sat. (1)	4
Sidgwick and Spurrell, 1920	273–298	sat. (32)	5
Wehrmann, 1921	263–303	sat. (33)	6
Perrakis, 1925	294	sat. (11)	7
Barbaudy, 1926	298	sat. (9)	8
Barbaudy, 1926	298–338	sat. (26), eq. (13)	9
Wright, 1926	284–296	sat. (7)	10
Barbaudy, 1927	338–342	eq. (6)	11
Washburn *et al.*, 1931	298	sat. (16), distr. (9)	12
Tarasenkov and Polozhentseva, 1932	293	eq. (6)	13
Sata and Kimura, 1935	303	sat. (7)	14
Varteressian and Fenske, 1936	298	sat. (10), eq. (14)	15
Bancroft and Hubard, 1942	298	sat. (4), eq. (12)	16
Staveley *et al.*, 1951	274–342	sat. (45)	17
Chang and Moulton, 1953	298	sat. (12), eq. (11)	18
Morachevskii and Belousov, 1958	293–337	eq. (35)	19
Mertslin *et al.*, 1961	299	sat. (20), distr. (12)	20
Ross and Patterson, 1979	293	eq. (9)	21
Brandani *et al.*, 1985	303–328	eq. (34)	22
Letcher *et al.*, 1990	298	sat. (13), eq. (5)	23

[a]Number of experimental points in parentheses.

Saturation curve

The ternary system ethanol–benzene–water forms a miscibility gap of type 1. Data for the system were reported in 23 references over the temperature range 263–342 K. The system is evaluated on the basis of the original papers. Only one binary system, benzene–water, is partially miscible. The data for this system were compiled and critically evaluated in a previously published SDS volume, Ref. 24. These recommended values of mutual solubility at 293 K are $x_2'=0.9975$, $x_2''=0.000\ 406$; at 298 K$-x_2'=0.9970$, $x_2''=0.000\ 409$ and at 333 K$-x_2'=0.991\ 04$, $x_2''=0.000\ 534$. Only the paper of Barbaudy, Ref. 9 at 333.2 K reported mutual solubility of the binary system: $x_2'=0.9893$ and $x_2''=0.0005$. This is in agreement with the recommended values, Ref. 24. The results of Taylor,[1] Lincon,[2] Perrakis,[7] Tarasenkov and Polozhentseva,[13] and Letcher *et al.*[23] are not reported as compilation tables. The data of Taylor[1] and Lincon[2] at 298.2 K published at 1896 and 1899, were reported as volume ratios. These data were recalculated to mole fractions, and they were taken into account for this evaluation; they are in agreement with other data sets at the same temperature. Data of Perrakis[7] at 294 K present a significantly larger miscibility gap than any other data at 293 K and therefore these data are rejected as are other alcohol–benzene–water systems presented in Ref. 7. Data of Tarasenkov and Polozhentseva[13] were obtained for this evaluation from Tarasenkov and Paulsen.[25] These data present a much smaller miscibility gap (at maximum ethanol concentration of about 0.03 mole fraction of C_2H_5OH) which is inconsistent with all other experimental data and an unreasonable large solubility of water in benzene (solubility of benzene in water estimated on the basis of these data seems to rech value $x_2''=0.94$). Therefore, this data set is rejected. All experimental data of Letcher *et al.*[23] were presented in the paper in graphical form only and therefore were not compiled. The miscibility gap decreased with the increasing temperature. This behavior is observed in all studies at more than one temperature.[5,6,9,17,19,22] Data reported by Brandani *et al.*[22] show a slightly smaller miscibility gap than other data at 303.2 K (Wehrmann, Ref. 6, and Sata and Kimura, Ref. 14) and at 313.2 K (Morachevskii and Belousov, Ref. 19). The reported data are consistent within each data set and for each study. All data on the saturation curve are treated as tentative. Characteristic points on the binodal curve at selected temperatures, reported or estimated for plait points and for maximum ethanol concentration, are presented in Table 18. At the point of maximum ethanol concentration the errors estimated by the evaluator are 0.005 and 0.015 mole fraction for ethanol and benzene, respectively.

TABLE 18. Characteristic points on the binodal curve of the system ethanol–benzene–water

	Max. C_2H_5OH concentration			Plait points		
T/K	x_1	x_2	Ref.	x_1	x_2	Ref.
288.2	0.438	0.198	3	0.389	0.413	3
293.2	0.435	0.195	6	-	-	
298.2	0.418	0.211	16	0.391	0.318	9
298.2	0.416	0.181	15	0.393	0.322	15
298.2	0.419	0.244	18	0.398	0.325	18
298.2	0.40	0.20	23	0.38	0.37	23
299.2	0.425	0.262	20	0.395	0.343	20
303.2	0.385	0.154	22	0.365	0.353	22
303.2	0.412	0.226	6	-	-	
313.2	0.384	0.198	19	0.344	0.330	22
328.2	0.354	0.271	22	0.354	0.271	22
338.2	0.344	0.212	9	0.344	0.212	9

The temperature of 298.2 K, a standard temperature in which various alcohol–hydrocarbon–water systems are presented, was chosen to present the behavior of the system. Saturation and equilibrium data of Refs. 1, 2, 5, 8, 9, 15, 16, and 18, water-rich and hydrocarbon-rich branches were described together by the equation:

$$x_1=0.541\,21+0.062\,76\ln(x_2)-0.083\,61x_2-0.468\,57x_2^2.$$

The least-squares method was used and the standard error of estimate was 0.0106. The proposed equation is not appropriate for the binodal curve at >0.98 mole fraction of benzene. The compositions on the saturation curve calculated by the proposed equation are presented in Table 19 for selected concentrations of benzene in the mixture. The results of the calculations (solid line) are also presented graphically in Fig. 10 together with selected experimental data, Refs. 5, 8, 9, 15, 16, 18, reported at 298.2 K.

TABLE 19. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 409 Ref. 24	0.3388	0.5000
0.1076	0.0010	0.3300	0.5200
0.2513	0.0100	0.3208	0.5400
0.2938	0.0200	0.3111	0.5600
0.3351	0.0400	0.3009	0.5800
0.3579	0.0600	0.2903	0.6000
0.3730	0.0800	0.2793	0.6200
0.3837	0.1000	0.2678	0.6400
0.3914	0.1200	0.2558	0.6600
0.3969	0.1400	0.2435	0.6800
0.4008	0.1600	0.2307	0.7000
0.4034	0.1800	0.2175	0.7200
0.4047	0.2000	0.2039	0.7400
0.4051	0.2200	0.1898	0.7600
0.4046	0.2400	0.1753	0.7800
0.4033	0.2600	0.1604	0.8000
0.4012	0.2800	0.1451	0.8200
0.3984	0.3000	0.1294	0.8400
0.3950	0.3200	0.1133	0.8600
0.3909	0.3400	0.0967	0.8800
0.3863	0.3600	0.0798	0.9000
0.3811	0.3800	0.0625	0.9200
0.3753	0.4000	0.0447	0.9400
0.3690	0.4200	0.0265	0.9600
0.3622	0.4400	0.0080	0.9800
0.3549	0.4600	0.0000	0.9970 Ref. 24
0.3471	0.4800		

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system ethanol–benzene–water were reported in 11 references over the temperature range 293–342 K as 20 data sets (mainly isotherms). The tie lines cover the full area of miscibility gap. Reported data are consistent within each data set. Only data of Tarasenkov and Polozhentseva[13] were rejected; these tie lines were inconsistent with all others. Vapor–liquid–liquid equilibria or boiling points of two-phase mixtures are reported in the papers of Barbaudy[11] at 101 kPa and of Morachevskii and Belousov[19] at temperatures 308.2, 318.2, 328.2, and 337.2 K. These data sets are consistent with other equilibrium data at lower temperatures. Changes of tie line direction are observed with temperature. With increasing temperature the water concentration in benzene-poor phase decreases for similar composition of benzene-rich phase; at temperatures over 333 K the concentration (in mole fraction) of ethanol in both phases in equilibrium reaches nearly the same values. This may be observed in data sets reported in Refs. 9, 11, 19, and 22. The equilibrium compositions of both phases of Ross and Patterson at 293.2 K[21] (referring also to density and surface tension of phases in equilibrium), are identical with those of Morachevskii and Belousov.[19] The reported experimental plait points are presented in Table 17. All equilibrium data are treated as tentative. Selected experimental points at 298.2 K, both saturation and equilibrium data, are presented in Fig. 10.

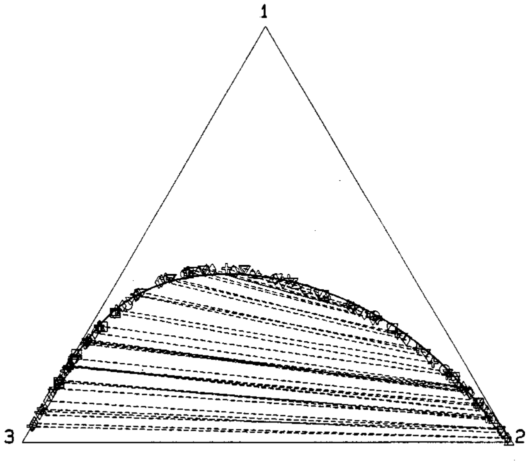

FIG. 10. Phase diagram of the system ethanol (1)—benzene (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 5, □—experimental data, Ref. 8, △—experimental data, Ref. 9, ◇—experimental data, Ref. 15, ✣—experimental data, Ref. 16, ▽—experimental data, Ref. 18, dashed lines—experimental tie lines. Refs. 9, 15, 16, and 18.

References:

[1] S. F. Taylor, J. Phys. Chem. **1**, 461 (1896–1897).
[2] A. T. Lincoln, J. Phys. Chem. **4**, 161 (1899–1900).
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[4] J. Holmes, J. Chem. Soc. **113**, 263 (1918).
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Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738-89 (1909-1910)

Variables:

$T/K = 273$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)
15.0	288.2	0.2165	0.7412	0.1453	0.8436
		0.3328	0.5166	0.2625	0.6910
		0.3886	0.4126	0.3333	0.6000 plait point
		0.4271	0.2906	0.4145	0.4783
		0.4381	0.1978	0.4784	0.3662
		0.4365	0.1409	0.5192	0.2841
		0.4251	0.1019	0.5430	0.2207
		0.4003	0.0759	0.5455	0.1755
		0.3854	0.0599	0.5475	0.1443
		0.3433	0.0360	0.5305	0.0944
		0.2920	0.0181	0.4929	0.0517
		0.1898	0.0038	0.3711	0.0126

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogenous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated Error:

accuracy of weighing 0.0001 g.

Components:	**Original Measurements:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) Benzene; C_6H_6; [71-43-2] (3) Water; H_2O; [7732-18-5]	N. V. Sidgwick and W. J. Spurrell, J. Chem. Soc. **117**, 1397–404 (1920).
Variables: T/K=272–312	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)
30.7	303.85	0.1496	0.8080	0.0974	0.8918
26.1	299.25	0.1698	0.7822	0.1121	0.8755
23.9	297.05	0.1781	0.7719	0.1182	0.8688
16.1	289.25	0.1974	0.7467	0.1329	0.8524
11.0	284.15	0.2084	0.7328	0.1414	0.8430
5.2	278.35	0.2212	0.7164	0.1515	0.8318
2.0	275.15	0.2283	0.7070	0.1572	0.8254
28.3	301.45	0.2978	0.5781	0.2245	0.7389
22.7	295.85	0.3074	0.5645	0.2338	0.7281
17.6	290.75	0.3177	0.5501	0.2440	0.7163
12.9	286.05	0.3286	0.5346	0.2550	0.7035
8.5	281.65	0.3404	0.5179	0.2672	0.6893
4.5	277.65	0.3529	0.5000	0.2805	0.6738
39.2	312.35	0.3428	0.4395	0.2922	0.6352
32.1	305.25	0.3547	0.4200	0.3071	0.6166
19.6	292.75	0.3805	0.3777	0.3411	0.5741
9.2	282.35	0.4188	0.3152	0.3961	0.5055
5.2	278.35	0.4363	0.2865	0.4234	0.4714
1.6	274.75	0.4507	0.2628	0.4470	0.4419
29.5	302.65	0.3985	0.2523	0.4139	0.4443
20.3	293.45	0.4227	0.2071	0.4601	0.3823
15.2	288.35	0.4338	0.1860	0.4832	0.3512
7.75	280.90	0.4480	0.1595	0.5138	0.3102
3.00	276.15	0.4550	0.1464	0.5296	0.2890
−1.25	271.90	0.4609	0.1353	0.5434	0.2704
25.3	298.45	0.4047	0.1322	0.4997	0.2767
21.2	294.35	0.4094	0.1220	0.5120	0.2588
17.3	290.45	0.4135	0.1134	0.5229	0.2431
13.5	286.65	0.4169	0.1058	0.5325	0.2291
9.9	283.05	0.4200	0.0992	0.5411	0.2167
6.5	279.65	0.4227	0.0934	0.5488	0.2055
1.95	275.10	0.4263	0.0857	0.5591	0.1906
15.4	288.55	0.3336	0.0402	0.5159	0.1053
12.15	285.30	0.3343	0.0382	0.5187	0.1005
7.1	280.25	0.3354	0.0350	0.5233	0.0925
2.3	275.45	0.3363	0.0322	0.5272	0.0856
−0.40	272.75	0.3367	0.0310	0.5289	0.0827
25.0	298.15	0.1994	0.0030	0.3861	0.0100

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)
0.0	273.2	0.2333	0.7008	0.1612	0.8210
		0.4561	0.2542	0.4559	0.4308
		0.4592	0.1385	0.5393	0.2759
		0.4277	0.0828	0.5631	0.1848
		0.3366	0.0312	0.5286	0.0832
1.0	274.2	0.2305	0.7044	0.1590	0.8235
		0.4531	0.2590	0.4510	0.4370
		0.4580	0.1407	0.5366	0.2795
		0.4270	0.0843	0.5611	0.1878
		0.3365	0.0317	0.5279	0.0844
2.0	275.2	0.2283	0.7073	0.1572	0.8255
		0.4493	0.2652	0.4446	0.4450
		0.4564	0.1438	0.5328	0.2846
		0.4262	0.0859	0.5589	0.1910
		0.3363	0.0322	0.5273	0.0855
3.0	276.2	0.2259	0.7103	0.1553	0.8276
		0.4448	0.2726	0.4372	0.4542
		0.4551	0.1461	0.5299	0.2885
		0.4254	0.0877	0.5564	0.1945
		0.3361	0.0327	0.5266	0.0868
4.0	277.2	0.2238	0.7130	0.1536	0.8295
		0.4411	0.2787	0.4311	0.4618
		0.4536	0.1490	0.5264	0.2932
		0.4247	0.0892	0.5544	0.1975
		0.3360	0.0332	0.5258	0.0881
5.0	278.2	0.2227	0.7145	0.1527	0.8305
		0.3508	0.5031	0.2782	0.6765
		0.4374	0.2847	0.4252	0.4692
		0.4520	0.1520	0.5228	0.2981
		0.4239	0.0909	0.5521	0.2008
		0.3358	0.0338	0.5250	0.0895
15.0	288.2	0.1997	0.7439	0.1346	0.8505
		0.3235	0.5418	0.2498	0.7095
		0.3944	0.3550	0.3604	0.5500
		0.4339	0.1858	0.4834	0.3510
		0.4158	0.1083	0.5293	0.2338
		0.3336	0.0399	0.5162	0.1047
25.0	298.2	0.1739	0.7771	0.1151	0.8722
		0.3036	0.5701	0.2300	0.7325
		0.3686	0.3972	0.3251	0.5941
		0.4109	0.2291	0.4370	0.4132
		0.4052	0.1310	0.5011	0.2746
		0.3305	0.0488	0.5039	0.1261
		0.1994	0.0030	0.3861	0.0100

Auxiliary Information

Method/Apparents/Procedur:

The apparatus consisted of Beckmann tube with air-jacket, thermometer and stirrer. Known amounts of aqueous alcohol mixture of known composition and benzene were placed in a tube. Aqueous alcohol mixtures were prepared gravimetrically. Components were added from an accurate pipette, which had been carefully graduated by weight. The reported temperatures (the mean of two or three observations) were those at which the liquid separated into two layers. The results, for the round temperatures, were interpolated by the authors from the curves. Concentrations were reported as alcohol mass concentration in alcohol–water mixture used in the experiment and benzene mass concentration in the solution which became turbid. The temperatures at which benzene crystallized from the investigated mixtures of know composition were reported also in the paper.

Source and Purity of Materials:

(1) source not specified, ordinary ''absolute'' alcohol; distilled from lime, water concentration was determined from the density using ''last edition of Beilstein's Handbuch der Organische Chemie,'' 99.5% alcohol was obtained by treatment with anhydrous copper sulphate and redistillation.
(2) source not specified; freed of thiophene by sulphuric acid, frozen out seven times, distilled over sodium.
(3) not specified.

Estimated Error:
Not reported.

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Meassurement:
F. Wehrmann, Z. Elektrochem. **27**, 379–93 (1921).

Variables:
T/K=263–303

Complied by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

		x_1	x_2	w_1	w_2
t/°C	T/K (compiler)	(compiler)		(compiler)	
−10	263.2	0.1846	0.0014	0.3653	0.0048
	263.2	0.3298	0.0142	0.5403	0.0394
	263.2	0.4115	0.0433	0.5895	0.1051
	263.2	0.4885	0.1010	0.5955	0.2088
	263.2	0.4579	0.3745	0.3953	0.5481
0	273.2	0.0347	0.0007	0.0839	0.0029
	273.2	0.1022	0.0009	0.2249	0.0035
	273.2	0.1781	0.0026	0.3541	0.0087
	273.2	0.2528	0.0081	0.4550	0.0247
	273.2	0.3176	0.0164	0.5242	0.0459
	273.2	0.3994	0.0538	0.5669	0.1295
	273.2	0.4702	0.1287	0.5562	0.2582
	273.2	0.3772	0.4810	0.3022	0.6534
	273.2	0.1035	0.8871	0.0642	0.9335
10	283.2	0.1785	0.0040	0.3534	0.0135
	283.2	0.3116	0.0191	0.5145	0.0534
	283.2	0.3948	0.0627	0.5536	0.1490
	283.2	0.4554	0.1573	0.5213	0.3053
	283.2	0.3416	0.5314	0.2643	0.6973
20	293.2	0.0346	0.0008	0.0837	0.0032
	293.2	0.1020	0.0024	0.2235	0.0089
	293.2	0.2501	0.0117	0.4477	0.0356
	293.2	0.3088	0.0262	0.5035	0.0725
	293.2	0.3890	0.0803	0.5310	0.1858
	293.2	0.4353	0.1845	0.4853	0.3489
	293.2	0.3150	0.5567	0.2406	0.7210
	293.2	0.0220	0.9760	0.0131	0.9864
30	303.2	0.0703	0.0021	0.1609	0.0083
	303.2	0.1772	0.0075	0.3483	0.0251
	303.2	0.3074	0.0316	0.4962	0.0866
	303.2	0.3869	0.0842	0.5252	0.1939
	303.2	0.4123	0.2257	0.4402	0.4086
	303.2	0.2890	0.6027	0.2135	0.7552

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Binary alcohol–water mixtures of known concentration and volume were put into Erlenmayer flasks, immersed in a constant temperature bath and then titrated with benzene until constant cloudiness was observed. Concentrations of alcohol–water mixtures were determined by density measurements. Results were reported in volume percentage.

Source and Purity of Materials:

(1) source not specified; chemically pure grade; used as received; d(15 °C)=0.8835.
(2) source not specified.
(3) not specified.

Estimated Error:
concentration ±0.3% relative error.

Components:	**Original Measurements:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2)Benzene; C_6H_6; [71-43-2] (3) Water; H_2O; [7732-18-5]	J. Barbaudy, Bull. Soc. Chim. Fr. **39**, 371–82 (1926).
Variables: T/K=298	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
25.00	298.15	0.4080	0.1360	0.4994	0.2823
		0.3112	0.0332	0.4988	0.0903
		0.2774	0.0241	0.4690	0.0691
		0.2100	0.0046	0.4000	0.0150
		0.3543	0.4403	0.3000	0.6320
		0.1442	0.0014	0.3000	0.0050
		0.2734	0.6206	0.2000	0.7697
		0.1551	0.8063	0.1009	0.8893
		0.0938	0.8861	0.0585	0.9366

Auxiliary Information

Method/Apparatus/Procedure:

The mixtures were prepared by weight (corrections on weighing in air were taken into account). Densities and refractive indexes of ternary liquid mixtures were measured. No further details were reported in the paper.

Source and Purity of Materials:

(1) source not specified; distilled over Na; d(25 °C,4 °C) $=0.785\ 06$, n(25 °C,D)$=1.3592$.
(2) Poluenc, without thiophene; b.p.=80.3 °C, d(25 °C,4 °C) $=0.873\ 63$, n(25 °C,D)$=1.497\ 95$.
(3) not specified.

Estimated Error:

Not reported.

Components:	**Original Measurements:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) Benzene; C_6H_6; [71-43-2] (3) Water; H_2O; [7732-18-5]	J. Barbaudy, Recl. Trav. Chim. Pays-Bas Belg. **45**, 207–13 (1926).
Variables: T/K=298–338	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
25.00	298.15	0.0000	0.9957	0.0000	0.9990
		0.0938	0.8857	0.0585	0.9365
		0.1553	0.8074	0.1009	0.8896
		0.2734	0.6206	0.2000	0.7697
		0.3543	0.4403	0.3000	0.6320
		0.4017	0.2825	0.4000	0.4770
		0.4080	0.1360	0.4994	0.2823
		0.3112	0.0332	0.4988	0.0903
		0.2742	0.0204	0.4690	0.0591
		0.2100	0.0046	0.4000	0.0150
		0.1442	0.0014	0.3000	0.0050
60.0	333.15	0.0000	0.0500	0.0000	0.1858
		0.1919	0.0126	0.3660	0.0407
		0.2287	0.0228	0.4083	0.0690
		0.2638	0.0381	0.4386	0.1074
		0.2977	0.0658	0.4523	0.1695
		0.3227	0.0856	0.4615	0.2076
		0.3413	0.1376	0.4385	0.2997
		0.3576	0.2187	0.4000	0.4147
		0.3566	0.2226	0.3968	0.4200
		0.3559	0.2254	0.3946	0.4238
		0.3531	0.3138	0.3477	0.5240
		0.3340	0.3944	0.3012	0.6030
		0.3180	0.4562	0.2695	0.6556
		0.2439	0.6329	0.1787	0.7861
		0.0000	0.9893	0.0000	0.9975

Compositions of coexisting phases

$t/°C$	T/K(compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.0226	0.9727	0.0766	0.0000	0.0135	0.9854	0.1750	0.0000
		0.0523	0.9376	0.1484	0.0016	0.0318	0.9658	0.3070	0.0055
		0.0856	0.9004	0.1819	0.0027	0.0529	0.9437	0.3600	0.0090
		0.3337	0.2946	0.4040	0.2698	0.3410	0.5105	0.4085	0.4625
		0.3914	0.3176	0.3914	0.3176	0.3750	0.5160	0.3750	0.5160[a]
65.0	338.15	0.2300	0.6727	0.2171	0.0190	0.1633	0.8097	0.3962	0.0587
		0.2314	0.6507	0.2224	0.0201	0.1676	0.7990	0.4023	0.0618
		0.3082	0.4864	0.2977	0.0667	0.2540	0.6798	0.4515	0.1715
		0.3437	0.3007	0.3384	0.1434	0.3463	0.5136	0.4315	0.3101
		0.3430	0.2970	0.3376	0.1488	0.3474	0.5100	0.4269	0.3191
		0.3490	0.2592	0.3397	0.1718	0.3706	0.4667	0.4132	0.3544
		0.3437	0.2547	0.3424	0.1735	0.3686	0.4630	0.4146	0.3562
		0.3438	0.2121	0.3438	0.2121	0.3920	0.4100	0.3920	0.4100[a]

[a] Plait point.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to find points on saturation curve. Samples of the binary benzene–ethanol mixture (30 mL at 25 °C and 10 mL in tubes with double walls and air jacket to eliminate heat transfer) were immersed in a thermostat, titrated with aqueous ethanol and refractive indexes were measured until the second phase appeared. The analytical method was used to determine coexisting phases. About 100–150 mL of mixture was placed in a 200 mL flask in a thermostat, agitated for more than 1 h, left for 8–48 h for separation and then density and refractive index of each phase were measured.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) source not specified.

Estimated Error:

Not reported.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. Wright, J. Chem. Soc. **129**, 1203–6 (1926).

Variables:

$T/K = 284–296$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
11.2	284.35	0.2767	0.0156	0.477 15	0.0457
13.2	286.35	0.2765	0.0164	0.4761	0.0478
15.5	288.65	0.2762	0.0173	0.474 75	0.0505
18.0	291.15	0.2760	0.0182	0.4735	0.0530
20.0	293.15	0.2758	0.0189	0.4726	0.0548
20.2	293.35	0.2757	0.0193	0.471 95	0.0561
22.6	295.75	0.2753	0.0206	0.470 15	0.0597

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Solubility was determined by adding a weighed quantity of benzene from a burette to a definite weight of alcohol–water mixture (about 12 g of 50% by weight of the aqueous alcohol) in a stoppered tube and raising the temperature until turbidity disappeared.

Source and Purity of Materials:

(1) not specified.
(2) not specified.
(3) not specified.

Estimated Error:

temp. ±0.1 °C.

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6 [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Meassurement:
J. Barbaudy, J. Chim. Phys. **24**, 1–23 (1927).

Variables:
T/K=338–342

Compiled by:
A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
69.0	342.15	0.0007	0.9865	0.0108	0.0007	0.0004	0.9966	0.027	0.003
68.0	341.15	0.0067	0.9805	0.0278	0.0010	0.0040	0.9930	0.068	0.004
67.0	340.15	0.0199	0.9631	0.0481	0.0012	0.0120	0.9840	0.114	0.005
66.0	339.15	0.0458	0.9333	0.0775	0.0016	0.0280	0.9670	0.176	0.006
65.5	338.65	0.0832	0.8881	0.1000	0.0019	0.0520	0.9410	0.220	0.007
65.0	338.15	0.1407	0.8198	0.1609	0.0059	0.0910	0.8990	0.324	0.020

Auxiliary Information

Method/Apparatus/Procedure:

Compositions of coexisting phases at boiling temperatures were determined as intersections of boiling isotherms in homogeneous and heterogeneous regions. Boiling temperatures were measured for over 100 ternary mixtures.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

Not reported.

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
E. R. Washburn, V. Hnizda, and R. Vold, J. Am. Chem. Soc. **53**, 3237–44 (1931).

Variables:
T/K=298

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
24.5	297.7	0.1287	0.8432	0.082	0.911
		0.1537	0.8070	0.100	0.890
		0.1925	0.7541	0.129	0.857
		0.2506	0.6564	0.179	0.795
		0.3235	0.5294	0.253	0.702
		0.3493	0.4571	0.291	0.646
		0.3804	0.3728	0.343	0.570
		0.4158	0.2723	0.416	0.462
		0.4161	0.2180	0.448	0.398
		0.4119	0.1345	0.504	0.279
		0.3991	0.1045	0.518	0.230
		0.3334	0.0438	0.512	0.114
		0.2692	0.0174	0.466	0.051
		0.1934	0.0064	0.374	0.021
		0.1441	0.0024	0.299	0.0083
		0.1203	0.0016	0.258	0.0057

Distribution of ethanol in ethanol–benzene–water system

t/°C	T/K (compiler)	w'_1 hydrocarbon-rich phase	w''_1 water-rich phase
25.0	298.2	0.007	0.025
		0.012	0.106
		0.016	0.164
		0.024	0.243
		0.039	0.318
		0.054	0.370
		0.070	0.405
		0.084	0.443
		0.098	0.573

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Binary alcohol–benzene mixtures of known composition, prepared from calibrated pipettes in 125 mL glass-stoppered bottles, were mixed, and titrated with water to a permanent cloudiness at room temperature (24.5 °C). The amount of water was 0.66–5.77 mL (added from a 10 mL burette graduated to 0.01 mL) and 17.1–112.7 mL (added from a calibrated 50 mL burette). The refractive indexes of mixtures were measured at 25.0 °C by Abbe refractometer and used to construct the plot of refractive index against composition which was further used to find compositions of equilibrium phases. Phase equilibrium data were reported in incomplete form. The mixtures of 25.0 mL of benzene and 25.0 mL of water were shaken and then suspended in the constant temperature bath to reach equilibrium. When the phases were transparent, refractive indexes of each layer were measured and compositions of the phases were calculated.

Source and Purity of Materials:

(1) standard commercial grade of absolute alcohol; dried with CaO and Ca until density measurements showed it to be better than 99.3%.
(2) Mallinckrodt, reagent quality; dried with Na, distilled.
(3) redistilled from $KMnO_4$.

Estimated Error:

temp. ±0.1 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

N. Sata and O. Kimura, Bull. Chem. Soc. Jpn. **10**, 409–20 (1935).

Variables:

$T/\mathrm{K}=303$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°\mathrm{C}$	T/K (compiler)	x_1 (compiler)	x_2	w_1 (compiler)	w_2
30	303.2	0.219	0.718	0.150	0.833
		0.350	0.459	0.291	0.647
		0.409	0.269	0.413	0.460
		0.403	0.132	0.498	0.277
		0.333	0.044	0.511	0.114
		0.232	0.010	0.426	0.031
		0.133	0.002	0.280	0.006

Auxiliary Information

Method/Apparents/Procedure:

Samples of known composition (by volume) were prepared in glass tubes (diameter—15 mm, length—200 mm) and sealed. These were placed in a thermostat and turbidity was observed after some (not reported) time. Eight series of measurements were made. The volume of alcohol was 2.00, 5.00, or 10.00 cm^3. The volume of second component was constant in the series, while the volume of the third component differed 0.05–0.02 cm^3 from point to point. The results were reported in the paper as the volumes of each component added into the tube.

Source and Purity of Materials:

(1) source not specified, 95% commercial reagent; purified with $KMnO_4$, refluxed 1 day with CaO, distilled; purity 99.53%, $d(25\ °\mathrm{C})=0.7865$.
(2) Merck, pure crystallized; distilled over Na.
(3) doubly distilled.

Estimated Error:

sol. ±0.01 cm^3 (authors), ±(0.0001–0.005) mass fraction (compiler).

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
K. A. Varteressian and M. R. Fenske, Ind. Eng. Chem. **28**, 928–33 (1936).

Variables:
T/K=298

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.15	0.0416	0.0002	0.0998	0.0010
		0.1150	0.0010	0.2488	0.0036
		0.1873	0.0033	0.3677	0.0111
		0.2761	0.0193	0.4724	0.0561
		0.3280	0.0399	0.5103	0.1052
		0.3572	0.0571	0.5230	0.1417
		0.3855	0.0860	0.5224	0.1976
		0.3930	0.3222	0.3740	0.5200
		0.3852	0.3418	0.3595	0.5409
		0.3086	0.5461	0.2390	0.7170

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.15	0.0101	0.9877	0.0471	0.0003	0.0060	0.9935	0.1120	0.0013
		0.0308	0.9628	0.0996	0.0007	0.0185	0.9800	0.2200	0.0028
		0.0576	0.9340	0.1496	0.0015	0.0350	0.9630	0.3090	0.0053
		0.0725	0.9150	0.1821	0.0030	0.0445	0.9525	0.3600	0.0102
		0.0733	0.9142	0.1849	0.0033	0.0450	0.9520	0.3640	0.0110
		0.1171	0.8586	0.2398	0.0109	0.0740	0.9200	0.4350	0.0335
		0.1192	0.8546	0.2453	0.0121	0.0755	0.9180	0.4410	0.0370
		0.1320	0.8360	0.2626	0.0162	0.0845	0.9075	0.4590	0.0480
		0.2034	0.7309	0.3539	0.0548	0.1385	0.8440	0.5220	0.1370
		0.2452	0.6631	0.3884	0.0898	0.1745	0.8000	0.5215	0.2045
		0.3162	0.5319	0.4150	0.1693	0.2475	0.7060	0.4800	0.3320
		0.3247	0.5115	0.4156	0.1813	0.2585	0.6905	0.4720	0.3490
		0.3489	0.4501	0.4126	0.2265	0.2930	0.6410	0.4400	0.4095
		0.393	0.322	0.393	0.322	0.374	0.520	0.374	0.520[a]

[a] Critical composition.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Refractive indexes were measured in saturation as well as equilibrium experiments.

Source and Purity of Materials:

(1) Barrett Co., thiophene-free, boiling range 1 °C: distilled, the middle portion was taken for the next distillation; b.p. =80.15 °C, $d(25\text{ °C},4\text{ °C})=0.8727$, $n(25\text{ °C,D})=1.4976$.
(2) U.S. Ind. Alcohol Co.; used as received; purity 99.8–99.9% by density measurements; b.p.=78.28 °C, $d(25\text{ °C},4\text{ °C})=0.7852$, $n(25\text{ °C,D})=1.3598$.
(3) doubly distilled; $n(25\text{ °C,D})=1.3326$.

Estimated Error:

temp. ±0.05 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bancroft and S. S. Hubard, J. Am. Chem. Soc. **64**, 347–53 (1942).

Variables:

T/K = 298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
25.0	298.2	0.1702	0.0032	0.3411	0.0109
		0.4105	0.1349	0.5025	0.2799
		0.3919	0.3509	0.3604	0.5471
		0.3246	0.5168	0.2570	0.6939

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.0101	0.9856	0.0382	0.0005	0.006	0.993	0.092	0.002
		0.0332	0.9583	0.0797	0.0005	0.020	0.978	0.181	0.002
		0.0586	0.9206	0.1298	0.0014	0.036	0.959	0.275	0.005
		0.0912	0.8842	0.1813	0.0039	0.057	0.937	0.358	0.013
		0.1294	0.8347	0.2354	0.0100	0.083	0.908	0.430	0.031
		0.1334	0.8269	0.2407	0.0111	0.086	0.904	0.436	0.034
		0.1609	0.7887	0.2789	0.0183	0.106	0.881	0.477	0.053
		0.1894	0.7462	0.3173	0.0337	0.128	0.855	0.505	0.091
		0.2244	0.6983	0.3551	0.0540	0.156	0.823	0.524	0.135
		0.2622	0.6355	0.3938	0.0958	0.190	0.781	0.521	0.215
		0.2934	0.5810	0.4106	0.1331	0.221	0.742	0.504	0.277
		0.3309	0.5030	0.4177	0.2105	0.265	0.683	0.454	0.388

Auxiliary Information

Method/Apparatus/Procedure:

The binodal curve was prepared by the titration method in glass-stoppered thermostated flasks. The end-point was taken as the first appearance of cloudiness (when water was the saturating liquid) and the first appearance of tiny drops (when benzene was the saturating liquid). The phase equilibrium data were obtained by the authors' new procedure described in the paper. A binary homogenous mixture of known composition was added to a known amount of the phase until homogenization was observed. Then the phase composition was calculated, by trial-and-error method, using the authors knowledge about binodal curve. Data reported in Refs. 1 and 2 were included in the description of the saturation curve.

Source and Purity of Materials:

(1) source not specified; absolute alcohol; dried with CaO, distilled.
(2) source not specified; thiophene-free grade; dried with CaO, distilled.
(3) distilled.

Estimated Error:

temp. ±0.1 °C.

References:

[1] A. T. Lincoln, J. Phys. Chem. **4**, 161 (1990)
[2] K. A. Varteressian and M. R. Fenske, Ind. Eng. Chem. **28**, 928 (1936).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. A. K. Staveley, R. G. S. Johns, and B. C. Moore, J. Chem. Soc. 2516–23 (1951).

Variables:

T/K = 274–342

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
27.2	300.35	0.006 44	0.990 44	0.003 82	0.995 46
34.4	307.55	0.006 44	0.989 60	0.003 82	0.995 26
42.2	315.35	0.006 44	0.988 27	0.003 82	0.994 95
53.7	326.85	0.006 44	0.985 54	0.003 83	0.994 30
55.2	328.35	0.006 44	0.985 05	0.003 83	0.994 19
66.5	339.65	0.006 44	0.981 37	0.003 84	0.993 31
14.7	287.85	0.0143	0.983 69	0.008 50	0.991 04
32.6	305.75	0.0143	0.981 60	0.008 51	0.990 54
37.4	310.55	0.0143	0.980 68	0.008 52	0.990 31
46.4	319.55	0.0143	0.978 73	0.008 53	0.989 84
51.6	324.75	0.0143	0.977 38	0.008 54	0.989 52
68.7	341.85	0.0143	0.971 42	0.008 58	0.988 07
26.1	299.25	0.0183	0.978 28	0.010 90	0.988 30
39.1	312.25	0.0183	0.976 145	0.010 92	0.987 78
45.4	318.55	0.0183	0.974 79	0.010 93	0.987 45
51.6	324.75	0.0183	0.973 43	0.010 94	0.987 12
60.6	333.75	0.0183	0.970 83	0.010 97	0.986 49
67.7	340.85	0.0183	0.968 64	0.010 99	0.985 95
18.7	291.85	0.024 65	0.971 77	0.014 73	0.984 44
23.1	296.25	0.024 65	0.971 16	0.014 73	0.984 29
26.6	299.75	0.024 65	0.970 67	0.014 74	0.984 17
32.1	305.25	0.024 65	0.969 78	0.014 75	0.983 95
41.6	314.75	0.024 65	0.968 25	0.014 77	0.983 57
57.3	330.45	0.024 65	0.965 76	0.014 80	0.982 95
61.7	334.85	0.024 65	0.964 09	0.014 82	0.982 54
68.4	341.55	0.024 65	0.962 60	0.014 83	0.982 17
16.7	289.85	0.029 86	0.965 43	0.017 89	0.981 00
32.3	305.45	0.029 86	0.963 13	0.017 93	0.980 43
43.4	316.55	0.029 86	0.961 76	0.017 95	0.980 08
55.6	328.75	0.029 86	0.959 61	0.017 98	0.979 54
11.5	284.65	0.042 13	0.951 91	0.025 40	0.973 19
27.9	301.05	0.042 13	0.949 60	0.025 45	0.972 60
38.6	311.75	0.042 13	0.948 25	0.025 48	0.972 25
38.8	311.95	0.042 13	0.948 17	0.025 48	0.972 23
39.0	312.15	0.042 13	0.947 83	0.025 48	0.972 14
62.1	335.25	0.042 13	0.943 25	0.025 58	0.970 95
1.3	274.45	0.0563	0.937 81	0.034 15	0.964 46
12.2	285.35	0.0563	0.935 95	0.034 20	0.963 96
27.5	300.65	0.0563	0.933 57	0.034 26	0.963 33
48.6	321.75	0.0563	0.928 93	0.034 39	0.962 08
13.0	286.15	0.0691	0.921 60	0.042 25	0.955 52
21.4	294.55	0.0691	0.919 78	0.042 31	0.955 02
32.6	305.75	0.0691	0.917 33	0.042 40	0.954 35
41.6	314.75	0.0691	0.914 30	0.042 50	0.953 51
56.5	329.65	0.0691	0.911 47	0.042 60	0.952 72

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Mixtures were prepared in sealed tubes; water was added from a weighted pipette to a known mass of alcohol–benzene mixture.

Source and Purity of Materials:

(1) source not specified; dried by refluxing over freshly ignited lime, and then with magnesium, distilled.
(2) source not specified; chemically purified, crystallized, distilled, dried over phosphoric anhydride.
(3) not specified.

Estimated Error:

composition <0.2%; temp. <0.2 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Y. C. Chang and R. W. Moulton, Ind Eng. Chem. **45**, 2350–61 (1953).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.1213	0.0012	0.2600	0.0043
		0.1496	0.0027	0.3080	0.0095
		0.1735	0.0038	0.3458	0.0129
		0.2737	0.0179	0.4711	0.0521
		0.3430	0.0486	0.5171	0.1242
		0.3978	0.1055	0.5160	0.2320
		0.4175	0.1639	0.4860	0.3235
		0.4177	0.2482	0.4310	0.4342
		0.3879	0.3617	0.3529	0.5580
		0.2947	0.5708	0.2241	0.7359
		0.2597	0.6379	0.1880	0.7830
		0.1508	0.8094	0.0980	0.8919

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.0310	0.9630	0.0676	0.0005	0.0186	0.9800	0.1561	0.0019
		0.0629	0.9233	0.1445	0.0018	0.0385	0.9582	0.3001	0.0065
		0.0994	0.8813	0.2001	0.0052	0.0621	0.9332	0.3850	0.0171
		0.1238	0.8425	0.2424	0.0094	0.0791	0.9125	0.4400	0.0288
		0.1671	0.7867	0.3097	0.0329	0.1100	0.8781	0.4975	0.0895
		0.2141	0.7181	0.3621	0.0621	0.1468	0.8350	0.5228	0.1521
		0.2542	0.6516	0.3964	0.1028	0.1821	0.7915	0.5172	0.2273
		0.2957	0.5788	0.4140	0.1423	0.2230	0.7400	0.4995	0.2911
		0.3081	0.5579	0.4176	0.1606	0.2358	0.7241	0.4885	0.3185
		0.3601	0.4268	0.4186	0.2439	0.3085	0.6201	0.4342	0.4289
		0.3980	0.3248	0.3980	0.3248	0.3765	0.5210	0.3765	0.5210[a]

[a] Plait point.

Auxiliary Information

Method/Apparatus/Procedure:

The cloud point method, as described in Ref. 1, was used. Binary alcohol–benzene mixtures were titrated with water to a sudden appearance of cloudiness. The end point was observed against a bright light as a background. Refractive indexes were measured at 25.5 °C with an Abbe refractometer. To obtain equilibrium, mixtures of known composition were overheated to about 35 °C and placed into a thermostat. When equilibrium was reached and the layers were clear in a bright light, phases were sampled, refractive indexes at 25.5 °C were measured and compositions were determined on the basis of charts obtained in saturation studies.

Source and Pority of Materials:

(1) source not specified, absolute alcohol; dehydrated by magnesium ethoxide method; b.p. = 78.3 °C; $n(25\ °\mathrm{C,D}) = 1.3596$; $d(25\ °\mathrm{C},4\ °\mathrm{C}) = 0.7851$.
(2) source not specified, reagent grade; dehydrated with Na wire, distilled; b.p. = 80.1 °C; $n(25\ °\mathrm{C,D}) = 1.4978$; $d(25\ °\mathrm{C},4\ °\mathrm{C}) = 0.8725$.
(3) distilled.

Estimated Error:

temp. ±0.1 °C (temperature of the bath), composition accuracy 0.5% in the center part of the binodal curve.

References:

[1] S. F. Taylor, J. Phys. Chem. **1**, 461 (1897).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. G. Morachevskii and V. P. Belousov, Vestn. Leningr. Univ., Ser. 4: Fiz. Khim. **4**, 117–25 (1958).

Variables:

T/K = 293–337

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_2'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20	293.2	0.3376	0.4941	0.4268	0.1971	0.272	0.675	0.470	0.368
		0.2809	0.6145	0.4180	0.1334	0.206	0.764	0.510	0.276
		0.2484	0.6786	0.3976	0.0941	0.174	0.806	0.526	0.211
		0.1633	0.7938	0.3179	0.0353	0.107	0.882	0.504	0.095
		0.1152	0.8565	0.2489	0.0118	0.073	0.920	0.446	0.036
		0.0762	0.9072	0.1881	0.0042	0.047	0.949	0.368	0.014
		0.0414	0.9501	0.1327	0.0017	0.025	0.973	0.280	0.006
		0.0118	0.9839	0.0637	0.0005	0.007	0.992	0.148	0.002
40	313.2	0.0201	0.9756	0.0642	0.0008	0.012	0.987	0.149	0.003
		0.0572	0.9261	0.1176	0.0016	0.035	0.961	0.253	0.006
		0.1062	0.8655	0.1792	0.0057	0.067	0.926	0.353	0.019
		0.1680	0.7929	0.2495	0.0184	0.110	0.880	0.440	0.055
		0.2550	0.6554	0.3273	0.0533	0.182	0.793	0.496	0.137
		0.3621	0.3801	0.3842	0.1979	0.327	0.582	0.435	0.380
60	333.2	0.0848	0.8866	0.1107	0.0022	0.053	0.940	0.240	0.008
		0.2118	0.7210	0.2300	0.0187	0.145	0.837	0.414	0.057
		0.2973	0.5312	0.3010	0.0527	0.235	0.712	0.468	0.139
		0.3393	0.3808	0.3424	0.0988	0.310	0.590	0.470	0.230

Compositions of coexisting phases (liquid–liquid–vapor-equilibria)

P/kPa	t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
			hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.6	35	308.2	0.014	0.982	0.056	0.001	0.0083	0.9907	0.1313	0.0040
28.3			0.080	0.899	0.154	0.003	0.0496	0.9453	0.3151	0.0104
28.8			0.145	0.816	0.241	0.015	0.0939	0.8962	0.4324	0.0456
29.2			0.197	0.746	0.298	0.033	0.1327	0.8522	0.4841	0.0909
28.9			0.255	0.649	0.348	0.064	0.1831	0.7900	0.5070	0.1581
28.5			0.320	0.508	0.386	0.124	0.2563	0.6898	0.4899	0.2669
39.7	45	318.2	0.017	0.979	0.051	0.001	0.0101	0.9889	0.1205	0.0040
44.8			0.086	0.889	0.140	0.003	0.0536	0.9403	0.2915	0.0106
45.9			0.156	0.801	0.217	0.012	0.1019	0.8871	0.4027	0.0378
46.1			0.213	0.727	0.270	0.027	0.1450	0.8390	0.4571	0.0775
45.9			0.270	0.619	0.320	0.053	0.1981	0.7701	0.4885	0.1372
60.3	55	328.2	0.023	0.972	0.044	0.001	0.0137	0.9851	0.1050	0.0040
67.3			0.092	0.879	0.124	0.003	0.0577	0.9352	0.2636	0.0108
68.8			0.164	0.789	0.195	0.010	0.1079	0.8800	0.3730	0.0324
69.7			0.222	0.704	0.250	0.022	0.1537	0.8263	0.4371	0.0652
69.4			0.278	0.586	0.300	0.047	0.2098	0.7500	0.4724	0.1255
84.5	64	337.2	0.020	0.971	0.037	0.001	0.0120	0.9859	0.0892	0.0041
95.7			0.099	0.873	0.108	0.002	0.0623	0.9309	0.2351	0.0074
97.6			0.174	0.776	0.172	0.008	0.1153	0.8718	0.3398	0.0268
98.5			0.228	0.685	0.235	0.020	0.1602	0.8159	0.4195	0.0605
98.4			0.284	0.563	0.280	0.042	0.2187	0.7352	0.4543	0.1155

Auxiliary Information

Method/Apparatus/Procedure:

Mixtures of known total composition were placed in a thermostat for about 2 h. After phase separation, samples of each phase were taken for analysis using heat-jacketed pipettes. Composition of each phase at different temperatures was found by determinations of the total amount of benzene in a sample combined with tie line data at 20 °C for the mixture investigated. Total amount of benzene was determined by adding a known amount of cyclohexane and 80% H_2SO_4. This caused separation to an acid–water–alcohol phase and a benzene–cyclohexane phase, the refractive index of which was measured. Benzene concentrations were calculated from the benzene–cyclohexane refractive index calibration curve. Tie lines at 20 °C were found by the method described above combined with the binodal curve data at 20 °C determined by isothermal titration method. Liquid–liquid equilibrium data were presented together with vapor pressure and vapor composition over two-liquid mixtures.

Source and Purity of Materials:

(1) source not specified; absolute alcohol was obtained by azeotropic dehydration with C_6H_6; $d(20\ °C,4\ °C)=0.7895$, $n(20\ °C,D)=1.3614$; in most of experiments distillate (containing water) was used; water concentration was determined densimetrically and taken into account in composition determinations.

(2) source not specified; pure for analysis grade, without thiophene; washed with H_2SO_4, H_2O, dried over $CaCl_2$, distilled; b.p. = 80.10 °C, $d(20\ °C,4\ °C)=0.8791$, $n(20\ °C,D)=1.5010$.

(3) not specified.

Estimated Error:

temp. $<\pm 0.1$ °C, error of analytical method $<0.5\%$.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. V. Mertslin, N. I. Nikurashina, and L. A. Kamaevskaya, Zh. Fiz. Khim. **35**, 2628–32 (1961).

Variables:

T/K = 299

Complied by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
26	299.2	0.1169	0.0014	0.2520	0.0050
		0.1873	0.0033	0.3677	0.0111
		0.2155	0.0066	0.4060	0.0210
		0.2738	0.0180	0.4710	0.0525
		0.3280	0.0399	0.5103	0.1052
		0.3569	0.0570	0.5228	0.1415
		0.3854	0.0857	0.5226	0.1970
		0.4052	0.1107	0.5180	0.2400
		0.4076	0.1167	0.5150	0.2500
		0.4107	0.1350	0.5026	0.2800
		0.4116	0.2140	0.4470	0.3940
		0.4247	0.2621	0.4283	0.4482
		0.3930	0.3222	0.3740	0.5200
		0.3950	0.3427	0.3662	0.5387[a]
		0.3706	0.4246	0.3166	0.6150
		0.3559	0.4590	0.2950	0.6450
		0.3086	0.5461	0.2390	0.7170
		0.3098	0.5619	0.2360	0.7258
		0.2629	0.6611	0.1860	0.7930
		0.1283	0.8397	0.0820	0.9100

[a] Critical solubility point.

Distribution of ethanol in ethanol–benzene–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_2'' water-rich phase
26	299.2	0.0660	0.0050
		0.1380	0.0100
		0.2150	0.0200
		0.2960	0.0300
		0.3780	0.0560
		0.4530	0.0800
		0.4930	0.1060
		0.5130	0.1380
		0.5230	0.1810
		0.5230	0.1810
		0.5200	0.2060
		0.5160	0.2180

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine the binodal curve. The refractive indexes of mixtures were measured at 26 °C using an IRF-22 refractometer to construct the calibration curve, which was then used to find the concentration of ethanol in both phases at equilibrium.

Source and Purity of Materials:

(1) source not specified, ‘‘absolute;’’ distilled; b.p.$=78.1$ °C, $n(26\ °\mathrm{C,D})=1.3596$.
(2) source not specified; doubly distilled; b.p.$=80.0$ °C, $n(26\ °\mathrm{C,D})=1.4975$.
(3) doubly distilled.

Estimated Error:

Not reported.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

S. Ross and R. E. Patterson J. Chem. Eng. Data **24**, 111–5 (1979).

Variables:

$T/\mathrm{K}=298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

$t/°\mathrm{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20.0	293.15	0.0000	1.0000	0.0000	0.0000	0.000	1.000	0.000	0.000
		0.0118	0.9839	0.0637	0.0005	0.007	0.992	0.148	0.002
		0.0414	0.9501	0.1327	0.0017	0.025	0.973	0.280	0.006
		0.0762	0.9072	0.1881	0.0042	0.047	0.949	0.368	0.014
		0.1152	0.8565	0.2489	0.0118	0.073	0.920	0.446	0.036
		0.1633	0.7938	0.3179	0.0353	0.107	0.882	0.504	0.095
		0.2484	0.6786	0.3976	0.0941	0.174	0.806	0.526	0.211
		0.2809	0.6145	0.4180	0.1334	0.206	0.764	0.510	0.276
		0.3376	0.4941	0.4268	0.1971	0.272	0.675	0.470	0.368

Auxiliary Information

Method/Apparatus/Procedure:

Mixtures of known composition (close to the midpoint) and mass of about 90 g were prepared by weighing into flasks with tightly fitting ground-glass stoppers. The solutions were shaken several times and placed in a thermostat for at least 24 h. Then density and surface tension of both phases as well as interfacial tension were measured.

Source and Purity of Materials:

(1) source not specified, absolute alcohol; dried with Mg, distilled; $\rho(20\ °\mathrm{C})=0.7895\ \mathrm{g\ cm^{-3}}$, b.p.$=77.9$–$78.1$ °C, $n(20\ °\mathrm{C,D})=1.3612$.
(2) source not specified, reagent grade; passed through a column of activated alumina into a bottle containing Na, distilled, (first and last portions of distillate were discarded); $\rho(20\ °\mathrm{C})=0.8792\ \mathrm{g\ cm^{-3}}$, b.p.$=79.6$–$79.8$ °C, $n(20\ °\mathrm{C,D})=1.5011$.
(3) distilled, redistilled from $KMnO_4$, acidified with phosphoric acid, redistilled, (all distillations under N_2 atmosphere).

Estimated Error:

temp. ±0.05 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. Brandani, A. Chianese, and M. Rossi, J. Chem. Eng. Data **30**, 27–9 (1985).

Variables:

T/K = 303–328

Complied by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
30.00	303.15	0.015	0.971	0.055	0.001	0.009	0.988	0.129	0.004
		0.053	0.935	0.133	0.003	0.032	0.965	0.279	0.011
		0.123	0.846	0.233	0.015	0.078	0.914	0.422	0.046
		0.138	0.816	0.243	0.015	0.090	0.899	0.435	0.046
		0.166	0.781	0.273	0.025	0.110	0.876	0.463	0.072
		0.194	0.725	0.315	0.039	0.133	0.845	0.497	0.104
		0.203	0.712	0.314	0.051	0.141	0.836	0.484	0.133
		0.242	0.662	0.343	0.082	0.173	0.801	0.485	0.197
		0.274	0.595	0.370	0.127	0.205	0.756	0.473	0.275
		0.288	0.555	0.376	0.162	0.223	0.729	0.452	0.330
		0.302	0.545	0.385	0.154	0.235	0.719	0.466	0.316
		0.302	0.526	0.377	0.179	0.239	0.707	0.441	0.355
		0.349	0.415	0.378	0.256	0.305	0.615	0.396	0.454
		0.365	0.353	0.365	0.353	0.340	0.557	0.340	0.557[a]
40.00	313.15	0.019	0.971	0.052	0.001	0.011	0.986	0.123	0.004
		0.065	0.918	0.129	0.004	0.040	0.956	0.272	0.014
		0.149	0.806	0.210	0.014	0.097	0.891	0.391	0.044
		0.163	0.776	0.233	0.016	0.108	0.876	0.421	0.049
		0.200	0.709	0.270	0.025	0.139	0.836	0.459	0.072
		0.228	0.674	0.305	0.039	0.162	0.811	0.486	0.105
		0.230	0.670	0.306	0.054	0.164	0.808	0.472	0.141
		0.265	0.592	0.324	0.094	0.200	0.758	0.456	0.224
		0.316	0.472	0.357	0.197	0.264	0.667	0.413	0.386
		0.324	0.436	0.356	0.237	0.280	0.639	0.388	0.438
		0.344	0.330	0.344	0.330	0.334	0.543	0.334	0.543[a]
55.00	328.15	0.026	0.960	0.046	0.002	0.016	0.981	0.109	0.008
		0.029	0.957	0.049	0.002	0.017	0.979	0.116	0.008
		0.094	0.875	0.125	0.005	0.059	0.933	0.264	0.018
		0.181	0.755	0.197	0.014	0.122	0.861	0.372	0.045
		0.183	0.747	0.209	0.017	0.124	0.858	0.387	0.053
		0.203	0.711	0.223	0.016	0.141	0.836	0.407	0.050
		0.241	0.643	0.256	0.024	0.175	0.792	0.443	0.070
		0.267	0.596	0.293	0.034	0.201	0.759	0.477	0.094
		0.268	0.581	0.287	0.060	0.204	0.751	0.446	0.158
		0.302	0.476	0.316	0.127	0.253	0.675	0.422	0.287
		0.344	0.351	0.343	0.151	0.325	0.562	0.430	0.321
		0.354	0.271	0.354	0.271	0.369	0.479	0.369	0.479[a]

[a] Plait point estimated by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Mixtures were stirred in an equilibrium cell fitted with a jacket for the circulating fluid and equipped with a mechanical stirrer. After equilibrium was reached each layer was withdrawn with a syringe and the composition was determined by glc (Carlo Erba Fractovap 2400 T, 2 m Poropak column, thermal conductivity detector; peak areas were measured with S-3380 Hewlett–Packard integrator). Calibration curves were prepared for the compositions closed to solubility curve at 20 °C. Each reported result is a mean of four analysis.

Source and Purity of Materials:

(1) source not specified, reagent grade; used as received.
(2) source not specified, reagent grade; used as received.
(3) doubly distilled.

Estimated Error:

temp. ±0.05 °C; composition accuracy ±1%.

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexene; C_6H_{10}; [110-83-8]
(3) Water; H_2O; [7732-18-5]

Evaluated by:
A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.05)

4.2. Ethanol + Water +Cyclohexene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system ethanol–cyclohexene–water is given in Table 20.

TABLE 20. Summary of experimental data for the system ethanol–cyclohexene–water

Author(s)	T/K	Type of data[a]	Ref.
Washburn *et al.*, 1940	298	sat. (12), eq. (6)	1
Kretschmer and Wiebe, 1945	228–298	sat. (9)	2

[a] Number of experimental points in parentheses.

Saturation curve

The system ethanol–cyclohexene–water forms a miscibility gap of type 1. Compositions along the saturation curves reported in both references were obtained by the titration method. Experimental data within each data set, measured at various temperatures, as well as both data sets, are consistent. The experimental results at 228, 273, and 298 K in the paper of Washburn *et al.*,[1] were expressed as the water tolerance of the alcohol–hydrocarbon mixture. Only one binary system, cyclohexene–water, forms a miscibility gap. Binary data of this system were compiled and critically evaluated in a previously published SDS volume.[3] The recommended, Ref. 3, values of mutual solubility at 298 K are: $x_2'=0.9983$ and $x_2''=0.000\,035$. Binary solubility data were not reported together with ternary data in any of the references discussed. Compositions of coexisting phases in equilibrium at 298.2 K, Ref. 1, are consistent with those measured along the saturation curve. Experimental results reported at lower temperatures by Kretschmer and Wiebe[2] are in agreement with the general expectation, at lower temperature the solubility gap increases. The maximum ethanol concentration is observed on the saturation curve at 298.2 K. It was reported to be $x_1=0.559$ and $x_2=0.157$.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system ethanol–cyclohexene–water were presented only in Ref. 1. The reported tie lines cover the whole range of miscibility gap. In the paper of Washburn *et al.*[1] two points reported for the hydrocarbon-rich phase did not contain water ($x_2=0.9947$ and $x_2=0.9460$). This presumably was the result of analytical limitations (self constructed refractive index–composition curve). Experimental compositions along the saturation curve and experimental compositions of coexisting phases in equilibrium at 298.2 K are treated as tentative and are presented in Fig. 11.

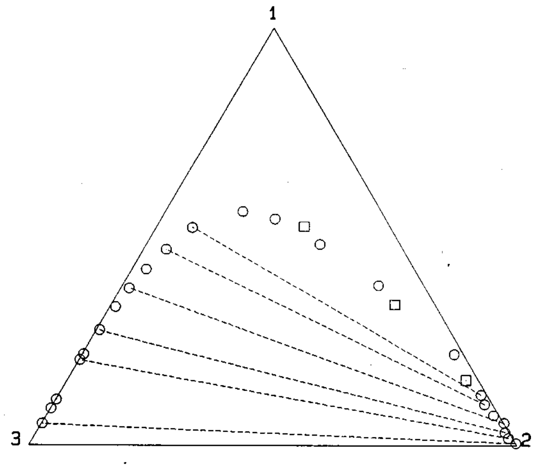

FIG. 11. Phase diagram of the system ethanol (1)—cyclohexene (2)—water (3) at 298.2 K. ○—experimental data, Ref. 1, □—experimental data, Ref. 2, dashed lines—experimental tie lines, Ref. 1.

References:

[1] E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transue, J. Am. Chem. Soc. **62**, 1454 (1940).

[2] C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130 (1945).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexene; C_6H_{10}; [110-83-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transue, J. Am. Chem. Soc. **62**, 1454–7 (1940).

Variables:

$T/\mathrm{K}=298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°\mathrm{C}$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.15	0.0727	0.9155	0.0425	0.9548
		0.2195	0.7607	0.1386	0.8565
		0.3827	0.5229	0.2831	0.6896
		0.4811	0.3537	0.4090	0.5361
		0.5415	0.2315	0.5192	0.3957
		0.5592	0.1570	0.5886	0.2946
		0.5213	0.0733	0.6431	0.1613
		0.4215	0.0285	0.6132	0.0739
		0.3313	0.0105	0.5454	0.0308
		0.2189	0.0017	0.4156	0.0059
		0.1098	0.0004	0.2394	0.0017
		0.0884	0.0003	0.1985	0.0012

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/°\mathrm{C}$	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.15	0.0053	0.9947	0.0521	0.0007	0.003	0.997	0.123	0.003
		0.0176	0.9734	0.2054	0.0009	0.010	0.988	0.397	0.003
		0.0314	0.9596	0.2762	0.0057	0.018	0.980	0.487	0.018
		0.0540	0.9460	0.3753	0.0166	0.031	0.969	0.584	0.046
		0.0992	0.8836	0.4689	0.0461	0.059	0.937	0.633	0.111
		0.1219	0.8653	0.5209	0.0731	0.073	0.924	0.643	0.161

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, as described in Ref. 1, was used. The titrant, from a weighed pipette, was added to the weighed binary mixture of known composition and the mixture was kept in a thermostated bath. To confirm that the end-point was reached the mixture was shaken automatically for at least 15 min and then reexamined. The plot of refractive index against composition was then used to find compositions of equilibrium phases. The refractive indexes were determinated at the temperature of 30.0 °C to eliminate an opalescence.

Source and Purity of Materials:

(1) Eastman Kodak Company, commercial grade; dried by refluxing over active lime, twice distilled; $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.7851$, $n(25\ °\mathrm{C},\mathrm{D})=1.359\,42$.
(2) Eastman Kodak Company, commercial grade; distilled in an atmosphere of purified N_2, collected in dried nitrogen-filled bottles; $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.8056$, $n(25\ °\mathrm{C},\mathrm{D})=1.4434$.
(3) not specified.

Estimated Error:

temp. ±0.05 °C.

References:

[1] E. R. Washburn and A. E. Beguin, J. Am. Chem. Soc. **62**, 579 (1940).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexene; C_6H_{10}; [110-83-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130–2 (1945).

Variables:

$T/\mathrm{K}=228-298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°\mathrm{C}$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)
−45.0	228.2	0.5967	0.3420	0.4849	0.4956
		0.3586	0.6166	0.2443	0.7491
		0.1610	0.8304	0.0979	0.9001
0.0	273.2	0.5531	0.3170	0.4731	0.4835
		0.3463	0.5954	0.2420	0.7420
		0.1593	0.8218	0.0976	0.8979
25.0	298.2	0.5234	0.3000	0.4643	0.4745
		0.3371	0.5797	0.2403	0.7366
		0.1581	0.8156	0.0974	0.8962

Comments and Additional Data

Water tolerance (S) was described with probable error $<0.5\%$ at the range −45–25 °C by the equation: $\log(S)=a-b/(T/\mathrm{K})$. The parameters (a,b) were determined from plots. Water tolerance was defined as: $S=H_2O\%$ by volume·(100 - Hydrocarbon % by volume in the blend)/100

vol % hydrocarbon	a	b
90	1.312	477.5
75	2.051	530.4
50	2.332	487.6

Auxiliary Information

Method/Apparatus/Procedure:

A glass tube with stirrer containing the ternary mixture was immersed in a bath, the temperature of which could be varied. Mixtures were prepared directly in the tube, by special pipettes at 15.5 °C. Precautions to exclude moisture and to prevent evaporation were observed. No correction was made for the slight expansion in volume when alcohol was mixed with hydrocarbon. In the paper the experimental results were expressed as the water tolerance of the alcohol–hydrocarbon blend. For practical purposes water tolerance was defined as the volume per cent of water which can be added before separation occurs.

Source and Purity of Materials:

(1) source not specified; anhydrous ethanol.
(2) source not specified; b.p. = 82.55–82.65 °C.
(3) not specified.

Estimated Error:

temp. within about 0.3 °C (duplicate determinations); composition $<0.2\%$ relative of volume fraction.

Components:	Evaluated by:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.04)

4.3. Ethanol + Water + Cyclohexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of ethanol between phases (distr.) for the system ethanol–cyclohexane–water is given in Table 21.

TABLE 21. Summary of experimental data for the system ethanol–cyclohexane–water

Author(s)	T/K	Type of data[a]	Ref.
Vold and Washburn, 1932	298	sat. (16), distr. (8)	1
Tarasenkov and Paulsen, 1937	273, 298	sat. (19)	2
Tarasenkov and Paulsen, 1939	298	eq. (3)	3
Kretschmer and Wiebe, 1945	228–298	sat. (5)	4
Connemann *et al.*, 1990	303–335	eq. (6)	5
Moriyoshi *et al.*, 1991	298, 323	eq. (36)	6
Letcher *et al.*, 1991	298	sat. (17), eq. (6)	7
Plackov and Stern, 1992	298	sat. (21), eq. (6)	8

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system ethanol–cyclohexane–water forms a miscibility gap of type 1. Eight studies of the system in the temperature range 228–335 K were reported; seven studies included measurements at 298 K. A growing saturation gap with the decreasing temperature is well observed from 298 to 335 K. The maximum ethanol concentration changes from 0.628 (298 K), through 0.598 (323 K) to 0.547 (335 K). The temperature 298.2 K was selected to present the behavior of the system. Only one binary system, cyclohexane–water, forms a miscibility gap. The data for this binary system were compiled and critically evaluated in a previously published SDS volume, Ref. 9; the recommended values of mutual solubility at 298.2 K are: $x_2''=1.2\cdot 10^{-5}$ and $x_3'=3.7\cdot 10^{-4}$.

The end points of saturation curve were reported to be pure cyclohexane and water.[6,7] For the water-rich phase and ethanol concentrations up to about 0.16 mole fraction the system was reported to be cyclohexane free.[6,7] All these results are within the accuracy of experimental measurements which were stated by the authors to be 0.001 mole fraction. The experimental point on saturation curve $x_2=0.0002$ by Vold and Washburn,[1] appears to contain experimental error and was rejected. All saturation data sets are consistent within each reference as well as with one another. Experimental solubility and equilibrium data reported at 298.2 K ($0.001<x_2<0.98$), for both water-rich and hydrocarbon-rich branches, were described by the equation:

$$x_1=1.021\,89+0.131\,29\ln(x_2)-1.019\,99x_2\,.$$

The least-squares method was used and the standard error of estimate was 0.0198. Compositions on the saturation curve calculated by this equation for selected concentrations of cyclohexane in the mixture are presented in Table 22 and in Fig. 12.

TABLE 22. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 012 Ref. 9	0.4209	0.5000
0.1140	0.0010	0.4056	0.5200
0.4071	0.0100	0.3902	0.5400
0.4879	0.0200	0.3746	0.5600
0.5585	0.0400	0.3588	0.5800
0.5913	0.0600	0.3428	0.6000
0.6087	0.0800	0.3267	0.6200
0.6176	0.1000	0.3105	0.6400
0.6211	0.1200	0.2941	0.6600
0.6210	0.1400	0.2777	0.6800
0.6181	0.1600	0.2611	0.7000
0.6132	0.1800	0.2444	0.7200
0.6066	0.2000	0.2276	0.7400
0.5987	0.2200	0.2107	0.7600
0.5897	0.2400	0.1937	0.7800
0.5798	0.2600	0.1766	0.8000
0.5692	0.2800	0.1594	0.8200
0.5578	0.3000	0.1422	0.8400
0.5459	0.3200	0.1249	0.8600
0.5335	0.3400	0.1075	0.8800
0.5206	0.3600	0.0901	0.9000
0.5073	0.3800	0.0725	0.9200
0.4936	0.4000	0.0550	0.9400
0.4796	0.4200	0.0373	0.9600
0.4653	0.4400	0.0196	0.9800
0.4507	0.4600	0.0000	0.999 63 Ref. 9
0.4359	0.4800		

Phases in equilibrium

Compositions of coexisting phases in equilibrium of the ternary system ethanol–cyclohexane–water were reported for the temperature range 298–335 K. The tie lines cover the full area of miscibility gap. The reported plait point calculated in Ref. 5 at 334.1 K was $x_1=0.437$ and $x_2=0.416$. Phase equilibrium data of Tarasenkov and Paulsen,[3] are inconsistent with saturation curve and are rejected. The other reported equilibrium data sets are consistent with one another, and within each data set. The small differences in tie lines are the result of experimental errors of phase analysis. The data for phases in equilibrium are considered tentative. The experimental tie lines at 298.2 K as well as all experimental points on saturation curve, Refs. 4, 6, 7 and 8, at 298.2 K, are reported in Fig. 12.

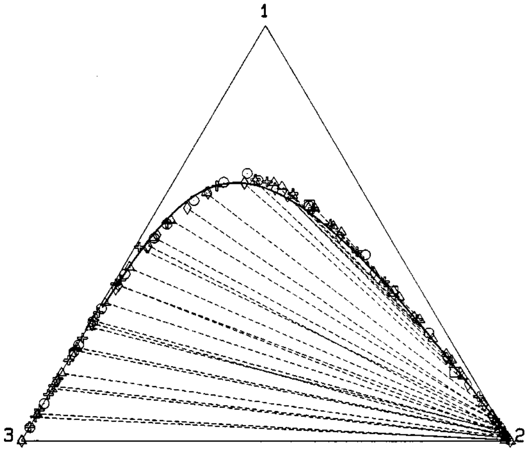

FIG. 12. Phase diagram of the system ethanol (1)—cyclohexane (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 1, □—experimental data, Ref. 4, △—experimental data, Ref. 6, ◇—experimental data, Ref. 7, ✙—experimental data, Ref. 8, dashed lines—experimental tie lines, Refs. 4, 6, 7, and 8.

References:

[1] R. D. Vold and E. R. Washburn, J. Am. Chem. Soc. **54**, 4217 (1932).

[2] D. N. Tarasenkov and I. A. Paulsen, Zh. Obshch. Khim. **7**, 2143 (1937).

[3] D. N. Tarasenkov and I. A. Paulsen, Acta Physicochim. URSS **9**, 75 (1939).

[4] C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130 (1945).

[5] M. Connemann, J. Gaube, L. Karrer, A. Pfennig, and U. Reuter, Fluid Phase Equilib. **60**, 99 (1990).

[6] T. Moriyoshi, Y. Uosaki, K. Takahashi, and T. Yamakawa, J. Chem. Thermodyn. **23**, 37 (1991).

[7] T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118 (1991).

[8] D. Plackov and I. Stern, Fluid Phase Equilib. **71**, 189 (1992).

[9] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:	**Original Measurements:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Water; H_2O; [7732-18-5]	R. D. Vold and E. R. Washburn, J. Am. Chem. Soc. **54**, 4217–25 (1932).
Variables:	**Compiled by:**
T/K=298	A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0314	0.0007	0.0763	0.0032
		0.0898	0.0014	0.2005	0.0059
		0.2143	0.0002	0.4106	0.0008
		0.2309	0.0016	0.4324	0.0054
		0.2868	0.0025	0.5038	0.0081
		0.3184	0.0044	0.5385	0.0136
		0.4014	0.0110	0.6163	0.0309
		0.4876	0.0278	0.6699	0.0698
		0.5213	0.0368	0.6847	0.0884
		0.5781	0.0634	0.6931	0.1388
		0.6226	0.1023	0.6789	0.2038
		0.6435	0.1399	0.6541	0.2598
		0.6269	0.1706	0.6159	0.3063
		0.5656	0.3056	0.4817	0.4754
		0.4485	0.4799	0.3314	0.6479
		0.2606	0.7039	0.1670	0.8241

Distribution of ethanol in ethanol–cyclohexane–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_1'' water-rich phase
25.00	298.15	0.000	0.0072
		0.000	0.0330
		0.000	0.0368
		—	0.0665
		0.0020	0.1274
		0.0037	0.1880
		0.0064	0.2810
		0.0120	0.4360

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to obtain points on the saturation curve. A 100 mL flask containing weighed amounts of ethanol and cyclohexane was suspended in a temperature controlled water bath at 24.8 °C and water was added from a weighed pipette until phase separation occurred. The appearance of a second phase was taken as the end-point. After each addition of water the flask was shaken for 30 s and then allowed to stand for at least 5 min. The flask was open only during addition of water from the pipette. The change of weight due to evaporation was no larger than 0.3%. Refractive index of each saturated mixture was measured at 25.0 °C, 0.2 °C above the titration temperature in order to assure homogeneous solutions. To determine the distribution of ethanol between water and organic phases, mixtures of 10 mL of water and different amounts of ethanol were prepared in glass-stoppered bottles, suspended in a thermostat 25.00 °C for 12 h and then the refractive indexes of both phases were measured and compared with those obtained for saturation mixtures.

Source and Purity of Materials:

(1) source not specified; absolute-standard commercial grade; refluxed over freshly ignited lime, distilled from an all-glass apparatus until density showed it to be 99.91% alcohol by Ref. 1.
(2) Eastman Kodak Co.; the best grade; fractionally crystallized, distilled, dried over Na, distilled; $\rho = 0.773\,79$ g/cm^3, f.p. $= 6.20$ °C.
(3) double distilled over $KMnO_4$.

Estimated Error:

temp. ±0.2 K (estimated by the compiler).

References:

[1] *International Critical Tables*, Vol. 3 (McGraw Hill, New York, 1929).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. N. Tarasenkov and I. A. Paulsen, Zh. Obshch. Khim. **7**, 2143–8 (1937).

Variables:

T/K = 273–298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
0.0	273.15	0.2316	0.7426	0.1449	0.8488
		0.3521	0.5680	0.2478	0.7302
		0.4245	0.5131	0.3062	0.6762
		0.6001	0.3085	0.5003	0.4699
		0.6636	0.1900	0.6214	0.3250
		0.6298	0.0699	0.7198	0.1460
		0.5971	0.0533	0.7184	0.1171
		0.4920	0.0182	0.6863	0.0465
		0.4288	0.0090	0.6447	0.0247
		0.3228	0.0040	0.5441	0.0122
		0.1682	0.0006	0.3402	0.0023
20.0	298.15	0.4477	0.4797	0.3310	0.6480
		0.5658	0.3056	0.4818	0.4754
		0.6110	0.2388	0.5524	0.3945
		0.6329	0.2050	0.5911	0.3497
		0.6357	0.1401	0.6491	0.2614
		0.6004	0.0773	0.6920	0.1627
		0.5212	0.0369	0.6845	0.0885
		0.3806	0.0075	0.6007	0.0217

Auxiliary Information

Method/Apparatus/Procedure:

A titration method similar to that in Ref. 1 was used. A flask of 100 mL capacity containing a binary cyclohexane–alcohol mixture of known composition, by weight, was placed in a thermostat. The mixture was titrated with water from a microburette with a scale of 0.01 mL, until opalescence, emulsion or turbidity was observed. Samples of the same binary composition were titrated several times.

Source and Purity of Materials:

(1) source not specified; purity of 99.97% for 3 points of the lower alcohol concentration at each temperature and purity of 92.64% for all other points.
(2) source not specified; distilled; b.p. = 80.9 °C, d(20 °C,4 °C) = 0.7744.
(3) source not specified.

Estimated Error:

temp. ±0.05 °C.

References:

[1] R. E. Washburn, J. Am. Soc. **53,** 3237 (1931).

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
D. N. Tarasenkov and I. A. Paulsen, Acta Physicochim. URSS **9**, 75–86 (1939).

Variables:
T/K=298

Compiled by:
A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.0110	0.9743	0.2530	0.0036	0.0061	0.9907	0.4598	0.0119
		0.0278	0.9563	0.3284	0.0044	0.0156	0.9809	0.5498	0.0135
		0.1607	0.7915	0.6135	0.1125	0.0989	0.8896	0.6624	0.2219

Auxiliary Information

Method/Apparatus/Procedure:
Not described. The data were also reported in Refs. 1 and 2.

Source and Purity of Materials:
(1) source not specified.
(2) source not specified.
(3) source not specified.

Estimated Error:
Not reported.

References:
[1] D. N. Tarasenkov and I. A. Paulsen, Zh. Obshch. Khim. **7**, 2143 (1937).
[2] D. N. Tarasenkov and I. A. Paulsen, Zh. Obshch. Khim. **8**, 76 (1938).

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130–2 (1945).

Variables:
T/K=298

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
−45.0	228.2	0.8347	0.1495	0.7493	0.2452[a]
0.0	273.2	0.6991	0.1252	0.7015	0.2295[a]
25.0	298.2	0.5680	0.3052	0.4834	0.4745
		0.3604	0.5809	0.2495	0.7346
		0.1662	0.8037	0.1010	0.8919

[a] Solution in equilibrium with solid cyclohexane.

Comments and Additional Data

Water tolerance (S) was described with probable error $< 0.5\%$ at the range −45–25 °C by the equation: $\log(S)=a-b/(T/\mathrm{K})$. The parameters ($a,b$) were determined from plots. Water tolerance was defined as: $S=H_2O$ % by volume·(100-Hydrocarbon % by volume in the blend)/100

vol % hydrocarbon	a	b
90	1.856	628.7
75	2.421	693.4
50	2.850	693.4
25	6.328	1526.0

at the range −45–0 °C; solution in equilibrium with solid cylohexane.

Auxiliary Information

Method/Apparatus/Procedure:
A glass tube with stirrer containing the ternary mixture was immersed in a bath, the temperature of which could be varied. Mixtures were prepared directly in the tube, by special pipettes at 15.5 °C. Precautions to exclude moisture and to prevent evaporation were observed. No correction was made for the slight expansion in volume when alcohol was mixed with hydrocarbon. In the paper the experimental results were expressed as the water tolerance of the alcohol–hydrocarbon blend. For practical purposes water tolerance was defined as the volume per cent of water which can be added before separation occurs.

Source and Purity of Materials:
(1) source not specified; anhydrous ethanol.
(2) source not specified; b.p.=78–81 °C.
(3) not specified.

Estimated Error:
temp. within about 0.3 °C (duplicate determinations); composition <0.2% relative of volume fraction.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. Connemann, J. Gaube, L. Karrer, A. Pfennig, and U. Reuter, Fluid Phase Equilib. **60**, 99–118 (1990).

Variables:

T/K = 303–335

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
30.0	303.2	0.027	0.969	0.337	0.004	0.015	0.984	0.560	0.012
61.4	334.6	0.074	0.910	0.424	0.019	0.042	0.954	0.627	0.051
60.5	333.7	0.146	0.826	0.521	0.080	0.088	0.906	0.633	0.178
61.6	334.8	0.200	0.757	0.547	0.140	0.125	0.864	0.591	0.276
61.5	334.7	0.316	0.601	0.515	0.262	0.218	0.759	0.476	0.443
60.9	334.1	0.437	0.416	0.437	0.416	0.348	0.606	0.348	0.606[a]

[a] Plait point evaluated by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

An equilibration cell with magnetic stirrer and a jacket for circulating thermostated fluid was used. Temperature was measured with a PT-100 resistance thermometer. After phase separation, samples of each phase were withdrawn with a syringe, dissolved in a known amount of 2-propanol and analyzed. Walter was determined by the Karl Fischer titration; the mass ratio of ethanol to cyclohexane was determined by glc using a peak-area calibration curve prepared earlier.

Source and Purity of Materials:

(1) Merck, Chromato-quality; dried over molecular sieves 3A; purity >99.8 mole %, impurities: organic <0.001 mass fraction, water <0.000 45 mass fraction by the Karl Fischer titration.
(2) Merck, Chromato-quality; dried over molecular sieves 3A; purity >99.8 mole %, impurities: organic <0.002 mass fraction, water <0.000 001 mass fraction by the Karl Fischer titration.
(3) distilled three times.

Estimated Error:

temp. ±0.1 K.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. Moriyoshi, Y. Uosaki, K. Takahashi, and T. Yamakawa, J. Chem. Thermodyn. **23**, 37–42 (1991).

Variables:

T/K = 298 and 323

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
		0.0020	0.9870	0.0640	0.0000	0.0011	0.9965	0.1488	0.0000
		0.0070	0.9840	0.1250	0.0000	0.0039	0.9942	0.2676	0.0000
		0.0110	0.9750	0.1640	0.0000	0.0061	0.9908	0.3341	0.0000
		0.0170	0.9750	0.2250	0.0010	0.0094	0.9888	0.4249	0.0035
		0.0260	0.9640	0.2740	0.0030	0.0145	0.9833	0.4874	0.0097
		0.0270	0.9630	0.3320	0.0050	0.0151	0.9827	0.5530	0.0152
		0.0380	0.9530	0.4180	0.0120	0.0213	0.9767	0.6306	0.0331
		0.0510	0.9440	0.4890	0.0260	0.0287	0.9702	0.6734	0.0654
		0.0630	0.9320	0.5310	0.0400	0.0356	0.9633	0.6880	0.0947
		0.0910	0.8980	0.5980	0.0790	0.0524	0.9451	0.6884	0.1661
		0.1570	0.8240	0.6250	0.1650	0.0940	0.9015	0.6197	0.2989
		0.1950	0.7830	0.6220	0.2050	0.1193	0.8754	0.5845	0.3519
		0.2210	0.7640	0.6130	0.2260	0.1305	0.8634	0.5630	0.3792
		0.2470	0.7180	0.5910	0.2590	0.1571	0.8342	0.5264	0.4214
		0.2930	0.6690	0.5600	0.3200	0.1915	0.7988	0.4700	0.4906
		0.3460	0.6010	0.5180	0.3790	0.2362	0.7496	0.4142	0.5536
		0.3620	0.5810	0.5030	0.4030	0.2504	0.7342	0.3942	0.5770
50.00	323.15	0.0000	1.0000	0.0000	0.0000	0.0000	1.0000	0.0000	0.0000
		0.0180	0.9820	0.1300	0.0000	0.0099	0.9901	0.2765	0.0000
		0.0260	0.9700	0.1820	0.0010	0.0144	0.9847	0.3616	0.0036
		0.0380	0.9600	0.2670	0.0030	0.0212	0.9784	0.4785	0.0098
		0.0480	0.9500	0.3210	0.0060	0.0269	0.9727	0.5394	0.0184
		0.0570	0.9400	0.3650	0.0080	0.0321	0.9672	0.5842	0.0234
		0.0620	0.9350	0.3920	0.0120	0.0350	0.9643	0.6059	0.0339
		0.0730	0.9230	0.4280	0.0210	0.0415	0.9577	0.6277	0.0563
		0.0760	0.9190	0.4480	0.0220	0.0433	0.9556	0.6442	0.0578
		0.0890	0.8990	0.4780	0.0370	0.0513	0.9460	0.6501	0.0919
		0.1250	0.8610	0.5470	0.0800	0.0734	0.9234	0.6520	0.1742
		0.1300	0.8540	0.5520	0.0850	0.0766	0.9197	0.6500	0.1829
		0.1580	0.8210	0.5780	0.1150	0.0948	0.9002	0.6365	0.2313
		0.1870	0.7820	0.5890	0.1230	0.1149	0.8777	0.6358	0.2426
		0.2300	0.7300	0.5980	0.1290	0.1456	0.8445	0.6359	0.2506
		0.2810	0.6620	0.5870	0.1740	0.1858	0.7995	0.5880	0.3184
		0.3800	0.5380	0.5530	0.2750	0.2724	0.7046	0.4926	0.4475
		0.4230	0.4830	0.5290	0.3230	0.3152	0.6574	0.4495	0.5014

Auxiliary Information

Method/Apparatus/Procedure:

The method was similar to that described in Ref. 1. After equilibrium was reached, both phases were analyzed by glc using acetone as an internal standard (a glass column (diameter 3.2 mm, 2 m long) packed with PEG-6000 Shimalite TPA; 353 K, He flow rate 0.33 mL/s). Compositions were determined from the peak-area diagram.

Source and Purity of Materials:

(1) source and purification procedure was described in Ref. 2.
(2) Dojin Chemical. Co.; spectrograde, used as received; refractive index agreed to within 0.005 with literature values.
(3) de-ionized, distilled over KMnO4, redistilled, by Ref. 1.

Estimated Error:

composition $<\pm 0.001$ mass fraction.

References:

[1] T. Moriyoshi, Y. Uosaki, H. Matsuura, and W. Nishimoto, J. Chem Thermodyn. **20**, 551 (1988).
[2] T. Moriyoshi, T. Sakamoto, and Y. Uosaki, J. Chem. Thermodyn. **27**, 947 (1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. Siswana, and S. E. Radloff, Afr. J. Chem. **44**, 118–21 (1991).

Variables:

T/k=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.144	0.001	0.300	0.004
		0.207	0.001	0.399	0.004
		0.280	0.004	0.494	0.013
		0.366	0.010	0.583	0.029
		0.466	0.024	0.657	0.062
		0.495	0.030	0.673	0.075
		0.597	0.083	0.683	0.174
		0.621	0.146	0.634	0.272
		0.607	0.215	0.568	0.367
		0.560	0.307	0.477	0.478
		0.492	0.404	0.387	0.581
		0.406	0.518	0.294	0.685
		0.298	0.655	0.197	0.791
		0.165	0.815	0.099	0.896
		0.088	0.903	0.051	0.947
		0.000	0.999	0.0000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C (compiler)	T/K	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.008	0.990	0.282	0.004	0.004	0.995	0.496	0.013
		0.015	0.982	0.374	0.012	0.008	0.991	0.588	0.034
		0.028	0.970	0.469	0.025	0.016	0.984	0.658	0.064
		0.061	0.930	0.560	0.059	0.035	0.963	0.686	0.132
		0.137	0.845	0.621	0.145	0.081	0.915	0.635	0.271
		0.200	0.770	0.590	0.249	0.124	0.869	0.533	0.411

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the titration method, as described in Ref. 1. The formation of a cloudy mixture was observed visually on shaking after addition of a known mass of the third component; syringes were precisely weighed. Tie line compositions were determined by the refractive index method,[2] and a complementary method using the Karl Fischer titration.[3] Measurements were made at pressure of 94.7 kPa.

Source and Purity of Materials:

(1) Merck: AR grade; refluxed with Mg and I_2, distilled; purity >99.9 mole % by glc.
(2) BDH; Gold label grade; used as received; purity >99.9 mole % by glc.
(3) not specified.

Estimated Error:

composition ±0.005 mole fraction (binodal curve), ±0.01 mole fraction (tie lines).

References:

[1] T. M. Letcher, S. Wooten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. Plackov and I. Stern, Fluid. Phase Equilib. **71**, 189–209 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.0433	0.9506	0.0243	0.9744
		0.1058	0.8826	0.0614	0.9360
		0.1890	0.7851	0.1157	0.8781
		0.2915	0.6653	0.1913	0.7976
		0.3824	0.5531	0.2697	0.7125
		0.4553	0.4600	0.3426	0.6324
		0.5204	0.3726	0.4187	0.5476
		0.5588	0.3181	0.4703	0.4891
		0.5945	0.2590	0.5285	0.4206
		0.6230	0.1915	0.5960	0.3347
		0.6284	0.1653	0.6215	0.2987
		0.6125	0.0939	0.6814	0.1908
		0.5235	0.0366	0.6867	0.0877
		0.3864	0.0105	0.6024	0.0299
		0.3073	0.0044	0.5258	0.0138
		0.2471	0.0021	0.4538	0.0070
		0.1931	0.0008	0.3788	0.0029
		0.1491	0.0005	0.3090	0.0019
		0.1111	0.0004	0.2419	0.0016
		0.0735	0.0002	0.1685	0.0008
		0.0334	0.0002	0.0811	0.0009

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25	298.2	0.003	0.994	0.057	0.000	0.002	0.998	0.134	0.000
		0.007	0.990	0.132	0.000	0.004	0.996	0.280	0.000
		0.015	0.982	0.218	0.003	0.008	0.991	0.413	0.010
		0.021	0.976	0.290	0.004	0.012	0.988	0.506	0.013
		0.032	0.964	0.377	0.005	0.018	0.981	0.601	0.015
		0.051	0.943	0.465	0.009	0.029	0.970	0.677	0.024

Auxiliary Information

Method/Apparatus/Procedure

Binodal compositions were determined by titration with the corresponding, less-soluble component until the appearance of turbidity, Ref. 1. The analytical method was used for determination of tie-lines. This was based on refractive indexes and densities of the samples, Ref. 1, combined with the oxidation of the alcohol with an excess of potassium dichromate and determination of unreduced dichromate with $Na_2S_2O_3$. Alcohol in the organic layer was determined after extraction with water.

Source and Purity of Materials:

(1) Kemika (Zagreb); analytical grade; presumably used as received; $n = 1.3593$, $\rho(25\ °C) = 787.0\ kg/m^3$, b.p. = 79.1 °C.
(2) Kemika (Zagreb); purity not specified; presumably used as received; $n = 1.4232$, $\rho(25\ °C) = 773.9\ kg/m^3$, b.p. = 80.0 °C.
(3) twice distilled in the presence of $KMnO_4$.

Estimated Error:

composition <0.0005 mass fraction, binodal, (relative); composition ±2%, tie line.

References:

[1] D. Plackov and I. Stern, Fluid Phase Equilib. **57,** 327 (1990).

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) 2,2-Dimethylbutane (neohexane); C_6H_{14}; [75-83-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130–2 (1945).

Variables:
$T/K = 228-298$

Compiled by:
A. Skrzecz

4.4. Ethanol + Water + 2,2-Dimethylbutane

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)
−45.0	228.2	0.6168	0.3178	0.4987	0.4806
		0.3824	0.5911	0.2552	0.7379
		0.1759	0.8158	0.1032	0.8949
0.0	273.2	0.5814	0.2996	0.4893	0.4716
		0.3713	0.5740	0.2532	0.7322
		0.1742	0.8078	0.1029	0.8929
25.0	298.2	0.5596	0.2883	0.4831	0.4656
		0.3640	0.5627	0.2519	0.7283
		0.1730	0.8021	0.1028	0.8914

Comments and Additional Data

Water tolerance (S) was described with probable error <0.5% at the range −45–25 °C by the equation: $\log(S) = a - b/(T/K)$. The parameters (a, b) were determined from plots. Water tolerance was defined as: $S = H_2O$ by volume·(100−Hydrocarbon % by volume in the blend)/100

vol % hydrocarbon	a	b
90	1.235	473.1
75	1.679	444.9
50	1.911	388.5

Auxiliary Information

Method/Apparatus/Procedure:

A glass tube with stirrer containing the ternary mixture was immersed in a bath, the temperature of which could be varied. Mixtures were prepared directly in the tube, by special pipettes at 15.5 °C. Precautions to exclude moisture and to prevent evaporation were observed. No correction was made for the slight expansion in volume when alcohol was mixed with hydrocarbon. In the paper the experimental results were expressed as the water tolerance of the alcohol–hydrocarbon blend. For practical purposes water tolerance was defined as the volume percent of water which can be added before separation occurs.

Source and Purity of Materials:

(1) source not specified; anhydrous ethanol.
(2) source not specified; b.p. = 49.7 °C.
(3) not specified.

Estimated Error:

temp. within about 0.3 °C (duplicate determinations), composition <0.2% relative of volume fraction.

Components:	**Evaluated by:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3] (3) Water (hydrogen oxide); H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.04)

4.5. Ethanol + Water + Hexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of ethanol between phases (distr.) for the system ethanol–hexane–water is given in Table 23.

TABLE 23. Summary of experimental data for the system ethanol–hexane–water

Author(s)	T/K	p/MPa	Type of data[a]	Ref.
Bonner, 1909	273		sat. (12)	1
Ormandy and Craven, 1922	242–304		sat. (25)	2
Tarasenkov and Paulsen, 1937	273, 298		sat. (25), eq. (2)	3
Mertslin *et al.*, 1961	293		sat. (8), distr. (18)	4
Vorobeva and Karapetyants, 1966	298		sat. (16), eq. (9)	5
Ross and Patterson, 1979	293		eq. (9)	6
Moriyoshi *et al.*, 1988	298	0.1–200	eq. (50)	7

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system ethanol–hexane–water forms a miscibility gap of type 1. The data are discussed on the basis of original papers with the exception of data of Ormandy and Craven,[2] which were taken from the handbook of Kafarov,[8] these data were also taken into account during evaluation but are not reported as compilation sheet because they do not contribute further to knowledge of the system. The influence of pressure over the range 0.1–200 MPa at 298 K was also studied;[7] the maximum concentration of ethanol on the saturation curve varies from $x_1 = 0.660$ at $p = 0.1$ MPa to $x_1 = 0.711$ at $p = 200$ MPa. Only the binary system hexane–water forms a miscibility gap. Data for this binary system were compiled and critically evaluated in a previously published SDS volume.[9] The values of mutual solubility of hexane–water system recommended at 298.2 K are: $x_2' = 2.3 \cdot 10^{-6}$ and $x_2'' = 0.999\,53$. The data of Tarasenkov and Paulsen at 273 and 298 K,[3] show larger miscibility gaps than any other data set; they are inconsistent and therefore rejected. The measurements of Vorobeva and Karapetyants,[5] and Ross and Patterson,[6] were made with the accuracy of 0.001 mass fraction, and therefore the reported solubilities of binary system hexane–water in these references are outlayers. One of experimental points measured by Mertslin *et al.*,[4] ($x_1 = 0.5582$, $x_2 = 0.3033$) is inconsistent and therefore is also rejected. Data of Bonner[1] measured at 273 K show a slightly larger immiscibility region which is in agreement with general expectation. A maximum value of ethanol concentration on the saturation curve of $x_1 = 0.66$ is observed at 298.2 K (Refs. 5 and 7). The temperature 298.2 K was selected to present the phase behavior; the data sets of Vorobeva and Karapetyants,[5] and Moriyoshi *et al.*[7] are consistent. These data were described by the equation:

$$x_1 = 1.04385 + 0.126\,03 \ln(x_2) - 1.046\,56\, x_2 .$$

The least-squares method was used and the standard error of estimate was 0.0165. Compositions on the saturation curve calculated by the proposed equation are presented in Table 24 for selected concentrations of hexane in the mixture. The results of calculations (solid line) are presented graphically in Fig. 13 together with experimental data reported at 298.2 K.

TABLE 24. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	$2.3 \cdot 10^{-6}$ Ref. 9	0.4172	0.5200
0.3709	0.0050	0.4010	0.5400
0.4530	0.0100	0.3847	0.5600
0.5299	0.0200	0.3682	0.5800
0.5963	0.0400	0.3515	0.6000
0.6265	0.0600	0.3347	0.6200
0.6418	0.0800	0.3178	0.6400
0.6490	0.1000	0.3008	0.6600
0.6510	0.1200	0.2836	0.6800
0.6495	0.1400	0.2663	0.7000
0.6454	0.1600	0.2489	0.7200
0.6393	0.1800	0.2314	0.7400
0.6317	0.2000	0.2139	0.7600
0.6228	0.2200	0.1962	0.7800
0.6128	0.2400	0.1785	0.8000
0.6020	0.2600	0.1607	0.8200
0.5904	0.2800	0.1428	0.8400
0.5781	0.3000	0.1248	0.8600
0.5653	0.3200	0.1068	0.8800
0.5521	0.3400	0.0887	0.9000
0.5383	0.3600	0.0705	0.9200
0.5242	0.3800	0.0523	0.9400
0.5097	0.4000	0.0340	0.9600
0.4950	0.4200	0.0157	0.9800
0.4799	0.4400	0.0065	0.9900
0.4646	0.4600	0.0019	0.9950
0.4490	0.4800	0.0000	0.99953 Ref. 9
0.4332	0.5000		

Phases in equilibrium

The phases in equilibrium were measured at 293 and 298 K over the pressure range 0.1–200 MPa. The tie lines of Ref. 3 are inconsistent and are rejected. The other tie lines cover the whole miscibility gap and are consistent within each data set, within each region and between the regions. The differences between compositions of the phases in equilibrium reported in Refs. 5 and 7 do not exceed 0.01 mole fraction. The solubility plait point of the system was reported only by Vorobeva and Karapetyants[5] at 298.2 K (($x_1 = 0.478$, $x_2 = 0.437$) and by Bonner[1] at 273.2 K ($x_1 = 0.498$, $x_2 = 0.414$). The experimental tie lines at 298.2 K are presented in Fig. 13 together with the saturation curve.

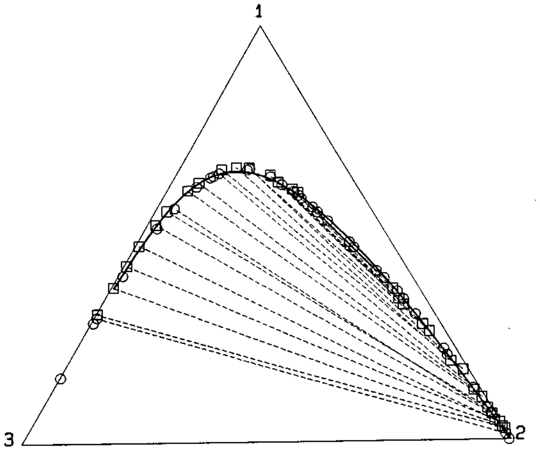

FIG. 13. Phase diagram of the system ethanol (1)—hexane (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental results of Ref. 5, □—experimental results of Ref. 7, dashed lines—experimental tie lines, Refs. 5 and 7.

References:

[1]W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).
[2]W. R. Ormandy and E. C. Craven, J. Inst. Petrol. Technol. **8**, 181, 213 (1922).
[3]D. N. Tarasenkov and I. A. Paulsen, Zh. Obshch. Khim. **7**, 2143 (1937).
[4]R. V. Mertslin, N. I. Nikurashina, and V. A. Petrov, Zh. Fiz. Khim. **35**, 2770 (1961).
[5]A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[6]S. Ross and R. E. Patterson, J. Chem. Eng. Data **24**, 111 (1979).
[7]T. Moriyoshi, Y. Uosaki, H. Matsuura, and W. Nishimoto, J. Chem. Thermodyn, **20**, 551 (1988).
[8]V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Part II (Izd. Akademii Nauk SSSR, Moskva, 1963).
[9]D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements;
W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910).

Variables:
T/K = 273

Complied by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)	
0.0	273.2	0.4978	0.4375	0.3711	0.6101	plait point
		0.5139	0.4142	0.3902	0.5884	
		0.6706	0.1893	0.6212	0.3280	
		0.6822	0.1588	0.6551	0.2853	
		0.6901	0.1112	0.7072	0.2132	
		0.6724	0.0810	0.7306	0.1646	
		0.6496	0.0557	0.7475	0.1199	
		0.6386	0.0484	0.7500	0.1062	
		0.5989	0.0327	0.7448	0.0761	
		0.5548	0.0202	0.7312	0.0497	
		0.4928	0.0121	0.6949	0.0320	
		0.2946	0.0021	0.5136	0.0068	

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogenous solution. The mass of binary water–hydrocarbon mixture was about 1 g the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled; $n(14\,°C) = 1.383\,82$.
(3) not specified.

Estimated Error:

accuracy of weighting 0.0001 g.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. N. Tarasenkov and I. A. Paulsen, Zh. Obshch. Khim. **7**, 2143–8 (1937).

Variables:

T/K=273–298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
0.0	273.15	0.1125	0.8536	0.0653	0.9270
		0.5730	0.3741	0.4430	0.5410
		0.6592	0.3000	0.5332	0.4539
		0.7371	0.2189	0.6334	0.3518
		0.7658	0.1199	0.7401	0.2167
		0.7310	0.0585	0.7922	0.1186
		0.6730	0.0364	0.7874	0.0796
		0.6715	0.0332	0.7908	0.0732
		0.6001	0.0167	0.7682	0.0400
		0.4897	0.0080	0.6985	0.0213
		0.4807	0.0058	0.6943	0.0157
		0.3745	0.0031	0.6004	0.0094
		0.2297	0.0012	0.4312	0.0042
25.0	298.15	0.0545	0.9014	0.0310	0.9592
		0.2843	0.6564	0.1852	0.7997
		0.4866	0.4420	0.3628	0.6164
		0.4971	0.4195	0.3782	0.5970
		0.6336	0.2994	0.5194	0.4591
		0.7321	0.1617	0.6803	0.2811
		0.7024	0.0896	0.7384	0.1761
		0.6602	0.0611	0.7473	0.1293
		0.5879	0.0342	0.7352	0.0800
		0.4709	0.0135	0.6749	0.0361
		0.3200	0.0059	0.5381	0.0186
		0.1870	0.0033	0.3668	0.0121

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.15	0.0015	0.9700	0.1916	0.0006	0.0008	0.9931	0.3767	0.0023
		0.0316	0.9434	0.3531	0.0097	0.0175	0.9771	0.5692	0.0291

Auxiliary Information

Method/Apparatus/Procedure:

A titration method similar to that in Ref. 1 was used. A flask of 100 mL capacity containing a binary hexane–alcohol mixture of known composition, by weight, was placed in a thermostat. The mixture was titrated with water from a microburette with a scale of 0.01 mL, until opalescence, emulsion or turbidity was observed. Samples of the same binary composition were titrated several times. Compositions of coexisting phases were obtained by an analytical method similar to that in Ref. 2. Experimental points were located on the binodal curve obtained by the authors. The ternary mixture became homogenous when the hexane concentration reached 79.4 mass % at 0 °C and 74.73 mass % at 25 °C.

Source and Purity of Materials:

(1) source not specified; purity of 99.97% for 3 points of the lower alcohol concentration at each temperature and purity of 92.64% for all other points.
(2) source not specified; distilled; b.p.=68.85 °C, d(20 °C,4 °C)=0.6898.
(3) source not specified.

Estimated Error:

temp. ±0.05 °C.

References:

[1] R. E. Washburn. J. Am. Soc. **53**, 3237 (1931).
[2] D. N. Tarasenkov and E. N. Polozhentseva, Zh. Obshch. Khim. **2**, 84 (1932)

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. V. Mertslin, N. I. Nikurashina, and V. A. Petrov, Zh. Fiz. Khim. **35**, 2770–4 (1961). [Eng. transl. Russ. J. Phys. Chem. **35**, 1369–72 (1961)].

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
20	293.2	0.3683	0.0048	0.5918	0.0143
		0.6543	0.0873	0.7122	0.1778
		0.6892	0.1224	0.6949	0.2308
		0.6327	0.2259	0.5697	0.3805
		0.5582	0.3033	0.4732	0.4809
		0.5054	0.4056	0.3891	0.5841
		0.4907	0.4234	0.3728	0.6017
		0.4824	0.4391	0.3615	0.6155

Distribution of ethanol in ethanol–hexane–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_1'' water-rich phase
20	293.2	0.2125	0.5675
		0.1325	0.6400
		0.0600	0.7300
		0.0200	0.6125
		0.0150	0.5650
		0.0125	0.5175
		0.0100	0.4775
		0.0075	0.4400
		0.0075	0.4125
		0.0060	0.3830
		0.0055	0.3625
		0.0055	0.3450
		0.0050	0.3250
		0.0050	0.3100
		0.0040	0.2925
		0.0040	0.2700
		0.0030	0.2550
		0.0030	0.2325

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine the binodal curve. The refractive indexes of mixtures were measured to construct the calibration curve, which was then used to find the concentration of ethanol in both phases at equilibrium.

Source and Purity of Materials:

(1) source not specified, dehydrated; distilled; b.p.=78.0 °C, n(20 °C,D)=1.3596.
(2) source not specified; doubly distilled; b.p.=68.5 °C, n(26 °C,D)=1.3751.
(3) doubly distilled.

Estimated Error:

Not reported.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018–23 (1966).
[Eng. transl. Russ. J. Phys. Chem. **40**, 1619–22 (1966)].

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Values

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9952	0.000	0.999
		0.2200	0.7548	0.134	0.860
		0.3391	0.6147	0.225	0.763
		0.465	0.4526	0.346	0.630
		0.5294	0.3677	0.421	0.547
		0.5915	0.2777	0.509	0.447
		0.6021	0.2630	0.525	0.429
		0.6378	0.1977	0.595	0.345
		0.6542	0.1415	0.655	0.265
		0.6393	0.0786	0.713	0.164
		0.6361	0.0735	0.717	0.155
		0.6141	0.0562	0.724	0.124
		0.5153	0.0233	0.697	0.059
		0.4007	0.0090	0.618	0.026
		0.2886	0.0040	0.504	0.013
		0.1588	0.0005	0.325	0.002

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.013	0.982	0.301	0.005	0.007	0.992	0.518	0.015
		0.065	0.926	0.562	0.036	0.036	0.962	0.714	0.086
		0.125	0.861	0.646	0.087	0.072	0.925	0.707	0.179
		0.205	0.769	0.657	0.145	0.124	0.870	0.653	0.270
		0.303	0.657	0.618	0.230	0.196	0.794	0.558	0.388
		0.358	0.593	0.584	0.287	0.241	0.746	0.499	0.458
		0.390	0.551	0.563	0.320	0.270	0.714	0.466	0.496
		0.408	0.526	0.551	0.336	0.288	0.694	0.450	0.514
		0.478	0.437	0.478	0.437	0.360	0.615	0.360	0.615

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, Ref. 1, was used to determine solubility of the mixtures. The third component was added to the binary homogenous mixture until cloudiness was first observed. Density of the saturated mixtures was measured; these results were graphed. To obtain equilibrium, ternary mixtures were stirred in a thermostated vessel for several hours. After phase separation, the density of each phase was measured and composition was determined from the graphs prepared earlier. Concentration at the critical point was found by method described in Ref. 2. Water included in ethanol was taken into account in all measurements.

Source and Purity of Materials:

(1) source not specified, ‘‘rectificate grade;’’ distilled; water concentration was determined by the Karl Fischer method.
(2) source not specified; b.p. = 68.7 °C, $n(20\ °\mathrm{C,D}) = 1.3753$.
(3) not specified.

Estimated Error:

solubility ±0.001 mass fraction.

References:

[1] W. D. Bancroft, Phys. Rev. **3**, 21 (1896).
[2] E. N. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

S. Ross and R. E. Patterson, J. Chem. Eng. Data **24**, 111–5 (1979).

Variables:

T/K = 298

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20.0	293.15	0.0000	1.0000	0.0000	0.0000	0.000	1.000	0.000	0.000
		0.0056	0.9944	0.1056	0.0000	0.003	0.997	0.232	0.000
		0.0093	0.9907	0.1586	0.0003	0.005	0.995	0.325	0.001
		0.0112	0.9888	0.1957	0.0005	0.006	0.994	0.383	0.002
		0.0149	0.9851	0.2358	0.0009	0.008	0.992	0.440	0.003
		0.0222	0.9778	0.2980	0.0018	0.012	0.988	0.518	0.006
		0.0368	0.9632	0.3914	0.0068	0.020	0.980	0.612	0.020
		0.1063	0.8892	0.5819	0.0349	0.060	0.939	0.730	0.082
		0.2170	0.7577	0.6710	0.1681	0.132	0.862	0.640	0.300

Auxiliary Information

Method/Apparatus/Procedure:

Mixtures of known composition (close to the midpoint) and mass of about 90 g were prepared by weighing into flasks with tightly fitting ground-glass stoppers. The solutions were shaken several times and placed in a thermostat for at least 24 h. Then density and surface tension of both phases as well as interfacial tension were measured.

Source and Purity of Materials:

(1) source not specified, absolute alcohol; dried with Mg, distilled; $\rho(20\ °\mathrm{C}) = 0.7895\ \mathrm{g\ cm^{-3}}$, b.p. = 77.9–78.1 °C, $n(20\ °\mathrm{C,D}) = 1.3612$.
(2) source not specified, reagent grade; passed through a column of activated alumina distilled, (first and last portions of distillate were discarded; $\rho(20\ °\mathrm{C}) = 0.6595\ \mathrm{g\ cm^{-3}}$, b.p. = 68.4–68.5 °C, $n(20\ °\mathrm{C,D}) = 1.3749$.
(3) distilled, redistilled from $KMnO_4$, acidified with phosphoric acid, redistilled, (all distillations under N_2 atmosphere).

Estimated Error:

temp. ±0.05 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. Moriyoshi, Y. Uosaki, H. Matsuura, and W. Nishimoto, J. Chem. Thermodyn. **20**, 551–7 (1988).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

			x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C (compiler)	T/K	p/MPa	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.00	298.15	0.1	0.026	0.974	0.310	0.001	0.014	0.986	0.533	0.003
			0.031	0.966	0.373	0.003	0.017	0.983	0.599	0.009
			0.042	0.956	0.425	0.005	0.023	0.977	0.647	0.014
			0.046	0.943	0.473	0.007	0.025	0.972	0.686	0.019
			0.062	0.930	0.523	0.017	0.034	0.964	0.712	0.043
			0.076	0.914	0.556	0.023	0.042	0.955	0.728	0.056
			0.102	0.890	0.605	0.042	0.058	0.941	0.736	0.096
			0.120	0.865	0.624	0.056	0.069	0.928	0.731	0.123
			0.170	0.818	0.655	0.088	0.100	0.898	0.712	0.179
			0.190	0.784	0.660	0.116	0.114	0.880	0.684	0.225
			0.262	0.705	0.659	0.143	0.164	0.828	0.656	0.266
			0.279	0.683	0.641	0.195	0.178	0.813	0.599	0.341
			0.326	0.621	0.624	0.220	0.216	0.770	0.569	0.375
			0.341	0.605	0.607	0.257	0.228	0.758	0.532	0.421
			0.364	0.581	0.599	0.272	0.247	0.738	0.517	0.439
		50	0.022	0.978	0.329	0.001	0.012	0.988	0.555	0.003
			0.038	0.959	0.450	0.006	0.021	0.979	0.668	0.017
			0.049	0.950	0.513	0.012	0.027	0.973	0.711	0.031
			0.064	0.930	0.558	0.019	0.035	0.963	0.735	0.047
			0.065	0.935	0.569	0.024	0.036	0.964	0.736	0.058
			0.074	0.916	0.603	0.034	0.041	0.957	0.746	0.079
			0.105	0.892	0.644	0.057	0.059	0.940	0.742	0.123
			0.208	0.775	0.674	0.131	0.125	0.871	0.677	0.246
			0.254	0.718	0.653	0.194	0.158	0.835	0.607	0.337
		100	0.019	0.978	0.346	0.001	0.010	0.989	0.574	0.003
			0.034	0.965	0.457	0.006	0.018	0.981	0.674	0.017
			0.036	0.964	0.515	0.011	0.020	0.980	0.714	0.029
			0.046	0.953	0.559	0.018	0.025	0.975	0.737	0.044
			0.057	0.943	0.589	0.025	0.031	0.969	0.749	0.059
			0.063	0.934	0.603	0.028	0.035	0.965	0.754	0.065
			0.076	0.912	0.643	0.043	0.043	0.955	0.760	0.095
			0.173	0.814	0.688	0.118	0.102	0.895	0.699	0.224
			0.203	0.779	0.677	0.160	0.122	0.874	0.651	0.288
			0.249	0.725	0.658	0.204	0.154	0.840	0.602	0.349
		150	0.024	0.974	0.456	0.004	0.013	0.987	0.676	0.011
			0.029	0.971	0.516	0.011	0.016	0.984	0.715	0.029
			0.039	0.961	0.559	0.016	0.021	0.979	0.740	0.040
			0.041	0.959	0.576	0.019	0.022	0.978	0.748	0.046
			0.046	0.954	0.605	0.026	0.025	0.975	0.758	0.061
			0.064	0.936	0.646	0.041	0.035	0.965	0.764	0.091
			0.176	0.813	0.692	0.145	0.103	0.894	0.674	0.264
			0.204	0.779	0.688	0.168	0.122	0.874	0.650	0.297
		200	0.015	0.975	0.411	0.002	0.008	0.990	0.638	0.006
			0.020	0.975	0.475	0.006	0.011	0.988	0.689	0.016
			0.023	0.975	0.512	0.010	0.012	0.987	0.713	0.026
			0.031	0.969	0.561	0.015	0.017	0.983	0.743	0.037
			0.056	0.932	0.649	0.036	0.031	0.966	0.773	0.080
			0.091	0.904	0.695	0.071	0.051	0.948	0.756	0.144
			0.151	0.839	0.711	0.126	0.088	0.910	0.704	0.233
			0.200	0.790	0.695	0.174	0.119	0.879	0.648	0.304

Auxiliary Information

Method/Apparatus/Procedure:

The experimental apparatus consisted of a high-pressure equilibrium cell, two hand operated pumps, a pressure exchanger, and two pressure gauges. The equilibrium cell, a stainless-steel cylinder of 50 cm^3 capacity, with mechanical stirrer was immersed in a thermostat. The mixtures, prepared by mass, were stirred under the desired conditions for at least 8 h and then allowed to settle for 2 h. Samples of each layer were withdrawn for glc analysis (glass column, 3.2 mm i.d ., 150 cm long, packed with PEG-6000 Shimalite F; T/K=343; thermal-conductivity detector equipped with electronic integrator). Acetone was used as an inert standard. Compositions were determined from the peak-area ratio and the calibration curve. Analysis of each phase were done at least twice.

Source and Purity of Materials:

(1) source not specified; dried by refluxing with CaO, followed by the Lund–Bjerrrum magnesium method, distilled.
(2) source not specified; shaken with conc. H_2SO_4, neutralized with aq. NaOH, dried over $CaCl_2$, distilled.
(3) de-ionized, distilled over $KMnO_4$, redistilled.

Estimated Error:

temp. ±0.002 K (control of the thermostat); press. ±0.1 MPa; composition ±0.003 mass fraction.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Evaluated by

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.05)

4.6. Ethanol + Water + Toluene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of ethanol between phases (distr.) for the system ethanol–toluene–water is given in Table 25.

TABLE 25. Summary of experimental data for the system ethanol–toluene–water

Author(s)	T/K	Type of data[a]	Ref.
Curtis, 1897	273	sat. (7)	1
Bonner, 1909	273	sat. (8)	2
Ormandy and Craven, 1921	243–303	sat. (48)	3
Tarasenkov and Polozhentseva, 1932	273–313	eq. (14)	4
Washburn *et al.*, 1939	298	sat. (17), distr. (9)	5
Leikola, 1940	293	sat. (8)	6
Mondain-Monval and Quiquerez, 1940	298	eq. (8)	7
Arzhanov *et al.*, 1975	348–357	eq. (6)	8
Borisova *et al.*, 1978	293–353	eq. (17)	9
Bevia *et al.*, 1985	298	sat. (10)	10
Ricna *et al.*, 1989	278–323	sat. (7), eq. (37)	11
Letcher and Siswana, 1992	298	sat. (15), eq. (6)	12

[a]Number of experimental points in parentheses.

Saturation curve

The ternary system ethanol–toluene–water forms a miscibility gap of type 1. There are 12 references for this system over the temperature range 243–353 K. This evaluation was made on the basis of original papers with the exception of data of Ormandy and Craven,[3] Tarasenkov and Polozhentseva,[4] and Leikola,[6] which were taken from the handbook of Kafarov;[13] these data were also taken into account during evaluation but are not reported as compilation sheet because they do not contribute further to knowledge of the system. Only the binary system toluene–water is partially miscible. The data for this system were compiled and critically evaluated in a previously published SDS volume.[14] The recommended values of mutual solubility at 298 K, are: $x_2'=0.9972$ and $x_2''=0.000\,0104$. The papers of Borisova *et al.*,[9] ($x_2'=0.9976$ and $x_2''=0.0001$ at 293.2 K) and Letcher and Siswana,[12] ($x_2'=0.999$ and $x_2''=0.000$ at 298.2 K) report mutual solubility of the binary system. Accuracy of experimental data reported in Ref. 12 was stated by the authors to be 0.005 mole fraction, so these data are consistent. The water-rich phase, Ricna *et al.*[11] is reported to be toluene free over a wide range of temperatures and water concentrations. This indicates that their experimental accuracy was in the range of 0.001–0.005 mole fraction; lower than reported (0.0001 mole fraction). Data of Arzhanov *et al.*[8] and Borisova *et al.*[9] reported for the temperature range 348–357 K describe the vapor–liquid–liquid equilibrium. (The boiling temperatures of two-phase mixture of Ref. 8 were estimated from authors graph.) The point ($x_1=0.5536$ and $x_2=0213$) on saturation curve at 278.2 K, Rican *et al.*[11] appears to contain a typing error and is rejected. Data reported for 273.2, 293.2, 313.2 K by Tarasenkov and Polozhentseva[4] contain errors for the toluene-rich phase; the experimental points are inconsistent with saturation curve in the region of low concentration of ethanol. These data are also rejected. Data of Borisova *et al.*,[9] at 293.2 K, close to the plait point, show a miscibility gap similar to the data at 273 K and larger than data of Leikola.[6] All other data for the saturation curve are consistent with one another. Ormandy and Craven[3] reported seven isotherms which clearly show the temperature dependence of the saturation data in the range 243–303 K. Characteristic points on the binodal curve of the system ethanol–toluene–water at selected temperatures, reported in literature, are presented in Table 26. At the maximum ethanol concentration point, the errors estimated by the evaluator are to be 0.005 and 0.015 mole fraction of ethanol and benzene, respectively.

TABLE 26. Characteristic points on the binodal curve of the system ethanol–toluene–water

	Max. C_2H_5OH concentration			Plait points		
T/K	x_1	x_2	Ref.	x_1	x_2	Ref.
243.2	0.573	0.168	3	—	—	
258.2	0.541	0.113	3	—	—	
273.2	0.523	0.143	3	—	—	
273.2	0.520	0.128	2	—	—	
278.2	0.512	0.161	3	—	—	
278.2	0.505	0.100	11	—	—	
288.2	0.493	0.193	3	—	—	
293.2	0.475	0.166	6	—	—	
293.2	0.503	0.197	9	0.464	0.357	9
298.2	0.474	0.123	3	0.423	0.341	7
298.2	0.473	0.127	11	—	—	
298.2	0.472	0.159	12	0.41	0.36	12
303.2	0.465	0.139	3	—	—	
323.2	0.425	0.160	11	—	—	
347.6	0.415	0.166	9	0.403	0.228	9
347.7	—	—		0.342	0.219	8

The temperature of 298.2 K was selected to present the behavior of the system. All experimental saturation and equilibrium points at 298.2 K water-rich and benzene-rich branches together, were described by the equation:

$$x_1=0.718\,83+0.092\,81\,\ln(x_2)-0.488\,76x_2-0.230\,41x_2^2.$$

The least-squares method was used and the standard error of estimate was 0.0125. The compositions on the saturation curve calculated by the proposed equation are presented in Table 27 for selected concentrations to toluene in the mixture. The results of calculations (solid line) are also presented graphically in Fig. 14 together with all experimental data reported at 298.2 K.

TABLE 27. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 0104 Ref. 14	0.3525	0.5000
0.0773	0.0010	0.3417	0.5200
0.2865	0.0100	0.3305	0.5400
0.3459	0.0200	0.3191	0.5600
0.4002	0.0400	0.3073	0.5800
0.4276	0.0600	0.2952	0.6000
0.4438	0.0800	0.2829	0.6200
0.4540	0.1000	0.2702	0.6400
0.4601	0.1200	0.2573	0.6600
0.4634	0.1400	0.2441	0.6800
0.4647	0.1600	0.2307	0.7000
0.4642	0.1800	0.2170	0.7200
0.4625	0.2000	0.2030	0.7400
0.4596	0.2200	0.1888	0.7600
0.4558	0.2400	0.1743	0.7800
0.4512	0.2600	0.1596	0.8000
0.4458	0.2800	0.1447	0.8200
0.4397	0.3000	0.1295	0.8400
0.4331	0.3200	0.1141	0.8600
0.4259	0.3400	0.0984	0.8800
0.4182	0.3600	0.0825	0.9000
0.4100	0.3800	0.0664	0.9200
0.4014	0.4000	0.0501	0.9400
0.3924	0.4200	0.0335	0.9600
0.3830	0.4400	0.0167	0.9800
0.3732	0.4600	0.0082	0.9900
0.3630	0.4800	0.0000	0.9972 Ref. 14

Phases in equilibrium

Compositions of the coexisting phases in equilibrium for the ternary system ethanol–toluene–water were reported in six references over the temperature range 273–357 K as 11 data sets. Two of these data sets, of Arzhanov *et al.*,[8] and Borisova *et al.*,[9] were measured at the boiling temperatures of two-phase mixtures at atmospheric pressure. Data reported by Tarasenkov and Polozhentseva[4] contain errors in the toluene-rich phase, as discussed above, and are rejected. Equilibrium phases for a boiling point of 248.2 K, Borisova *et al.*[9] contain presumably an analytical error. This tie line is inconsistent within the data set; other tie lines at boiling temperatures, Refs. 8 and 9, are consistent and cover the full miscibility gap. Other reported data are consistent within each data set. The distribution of ethanol (direction of tie lines) between the phases changes with temperature and at the boiling point (348–357 K) the concentration of ethanol in both phases becomes nearly the same. The reported plait points are presented above in Table 2. All equilibrium data are treated as tentative. All experimental points at 298.2 K, both saturation and equilibrium data,[3,5,7,10,11,12] are presented in Fig. 14.

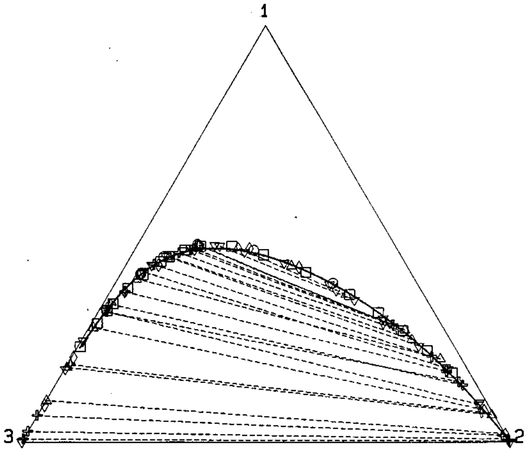

FIG. 14. Phase diagram of the system ethanol (1)—toluene (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ◇—experimental data, Ref. 10, ○—experimental data, Ref. 3, ✣—experimental data, Ref. 11, □—experimental data, Ref. 5, ▽—experimental data, Ref. 12, △—experimental data, Ref. 7, dashed lines—experimental tie lines, Refs. 7, 11, and 12.

References:

[1] C. B. Curtis, J. Phys. Chem. **2**, 371 (1897–1898).

[2] W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).

[3] W. R. Ormandy and E. C. Craven, J. Inst. Pet. Technol. **7**, 325, 422 (1921).

[4] D. N. Tarasenkov and E. N. Polozhentseva, Zh. Obshch. Khim. **2**, 84 (1932).

[5] R. E. Washburn, A. E. Beguin, and O. C. Beckord, J. Am. Chem. Soc. **61**, 1694 (1939).

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[7] P. Mondain-Monval and J. Quiquerez, Bull. Soc. Chim. Fr., Mem. **7**, 240 (1940).

[8] P. G. Arzhanov, L. F. Komarova, and Yu. N. Garber, Zh. Prikl. Khim. (Leningrad) **48**, 2089 (1975).

[9] I. A. Borisova, V. G. Vatskova, A. I. Gorbunov, and N. M. Sokolov, Khim. Prom-st (Moscow) 347 (1978).

[10] F. R. Bevia, D. P. Rico, and V. G. Yagues, Fluid Phase Equilibria **23**, 269 (1985).

[11] K. Ricna, J. Matous, J. P. Novak, and V. Kubicek, Collect. Czech. Chem. Commun. **54**, 581 (1989).

[12] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

[13] V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Part II (Izd. Akademii Nauk SSSR, Moskva, 1963).

[14] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 Pergamon, New York, 1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910).

Variables:

T/K = 273

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)
0.0	273.2	0.3900	0.4764	0.2795	0.6830
		0.4451	0.3793	0.3498	0.5962
		0.4849	0.3023	0.4135	0.5155
		0.5198	0.1275	0.5695	0.2794
		0.4937	0.0748	0.6080	0.1842
		0.4202	0.0339	0.5990	0.0966
		0.3831	0.0226	0.5798	0.0685
		0.3224	0.0098	0.5345	0.0326
		0.2463	0.0042	0.4496	0.0154

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogenous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated Error:

accuracy of weighing 0.0001 g.

Components:	**Original Measurements:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) Toluene (methylbenzene); C_7H_8; [108-88-3] (3) Water; H_2O; [7732-18-5]	R. E. Washburn, A. E. Beguin, and O. C. Beckord, J. Am. Chem. Soc. **61**, 1694–5 (1939).
Variables: T/K=298	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.1662	0.7975	0.0936	0.8984
		0.2194	0.7195	0.1304	0.8554
		0.2668	0.6464	0.1674	0.8113
		0.3106	0.5737	0.2066	0.7633
		0.3543	0.4935	0.2529	0.7046
		0.4074	0.3780	0.3266	0.6061
		0.4497	0.2712	0.4083	0.4926
		0.4695	0.1952	0.4737	0.3940
		0.4696	0.1310	0.5289	0.2952
		0.4604	0.1033	0.5496	0.2467
		0.4449	0.0787	0.5642	0.1996
		0.4333	0.0674	0.5676	0.1766
		0.4022	0.0459	0.5666	0.1294
		0.3697	0.0314	0.5546	0.0941
		0.3315	0.0199	0.5304	0.0637
		0.3155	0.0162	0.5178	0.0533
		0.2843	0.0108	0.4889	0.0372
		0.2284	0.0047	0.4248	0.0175

Distribution of ethanol in ethanol–toluene–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_1'' water-rich phase
25.0	298.2	0.002	0.110
		0.007	0.192
		0.013	0.257
		0.027	0.352
		0.047	0.417
		0.053	0.469
		0.065	0.500
		0.082	0.533
		0.094	0.556

Auxiliary Information

Method/Apparatus/Procedure:

The solubility curve was determined in a constant temperature bath by a titration method similar to that reported in Refs. 1–3. Refractive indexes were measured with an Abbe refractometer at the same temperature and presented as a concentration function in a graph. This graph was used to determine the concentration of alcohol in the samples of each phase when equilibrium had been reached. Phase equilibrium data were reported only as distribution of ethanol.

Source and Purity of Materials:

(1) source not specified; commercial grade absolute ethanol; refluxed over lime, distilled; $d(25\ °C,4\ °C)=0.7851$, $n(25\ °C,D)=1.359\ 40$.
(2) source not specified; analytical reagent grade; dried over Na, distilled; $d(25\ °C,4\ °C)=0.8608$, $n(25\ °C,D)=1.493\ 71$.
(3) distilled over $KMnO_4$.

Estimated Error:

temp. ±0.1 °C.

References:

[1] E. R. Washburn, V. Hnizda, and R. Vold, J. Am Chem. Soc. **53**, 3237 (1931).
[2] R. Vold and E. R. Washburn, J. Am. Chem. Soc. **54**, 4217 (1932).
[3] E. R. Washburn and H. C. Spencer, J. Am. Chem. Soc. **56**, 361 (1934).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Toluene (methylbenzene); C_7H_8 ; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. Mondain-Monaval, and J. Quiquerez, Bull. Soc. Chim. Fr., Mem. **7**, 240–53 (1940).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (complier)		water-rich phase (complier)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.020	0.980	0.0994	0.0002	0.010	0.990	0.220	0.001
	298.15	0.066	0.930	0.179	0.002	0.034	0.965	0.355	0.009
	298.15	0.078	0.908	0.274	0.008	0.041	0.956	0.480	0.029
	298.15	0.199	0.757	0.391	0.038	0.115	0.875	0.566	0.111
	298.15	0.246	0.675	0.445	0.079	0.151	0.830	0.564	0.200
	298.15	0.269	0.649	0.472	0.127	0.168	0.812	0.535	0.287
	298.15	0.354	0.486	0.466	0.210	0.255	0.700	0.460	0.415
	298.15	0.423	0.341	0.423	0.341	0.353	0.570	0.353	0.570[a]

[a] Plait point.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. A sample of 100 mL of a ternary mixture, prepared by weight, was placed in a thermostat, agitated many times and then left for several hours to separate. The density and refractive index of each phase was measured. Inversion of density was observed.

Source and Purity of Materials:

(1) source not specified; d(25 °C,4 °C)=0.7853.
(2) obtained in the laboratory; d(24 °C,4 °C)=0.8622.
(3) not specified.

Estimated Error:

temp. ±0.02 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. G. Arzhanov, L. F. Komarova, and Yu. N. Garber, Zh. Prikl. Khim. (Leningrad) **48**, 2089–91 (1975). [Eng. transl. Russ. J. Appl. Chem. (Leningrad) **48**, 2160–2 (1975)].

Variables:

T/K=348–353

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
80.0	353.2	0.075	0.925	0.085	0.000	0.039	0.961	0.192	0.000
76.5	349.7	0.139	0.815	0.144	0.003	0.078	0.912	0.298	0.012
75.5	348.7	0.205	0.705	0.220	0.006	0.124	0.854	0.412	0.022
75.1	348.3	0.261	0.603	0.263	0.015	0.172	0.793	0.457	0.052
74.7	347.9	0.290	0.530	0.283	0.030	0.204	0.746	0.463	0.098
74.5	347.7	0.342	0.219	0.342	0.219	0.359	0.460	0.359	0.460

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The equilibrium was investigated at the boiling temperature at 760 Torr. The samples were taken for glc analysis through heated capillaries. Analysis: column 2 m long and 4 mm diameter filled with polichrom with 15% polyethyleneglycoladipinate; 100 °C; H_2 100 mL/min; internal standard and homogenizer–acetone. Boiling temperatures of the two-phase mixture at 760 Torr were estimated from the authors' graph.

Source and Purity of Materials:

(1) Source not specified; purified in the laboratory; b.p.=78.3 ±0.1 °C, n(20 °C,D)=1.3614; the properties were in agreement with literature data, purity was checked by glc analysis.
(2) source not specified; purified in the laboratory; b.p.=110.7 ±0.1 °C, n(20 °C,D)=1.4969; the properties were in agreement with literature data, purity was checked by glc analysis.
(3) double distilled.

Estimated Error:

pressure ±0.1 Torr.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Toluene (methylbenzene); C_7H_8 ; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

I. A. Borisova, V. G. Vatskova, A. I. Gorbunov, and N. M. Sokolov, Khim. Prom-st (Moscow) 347 (1978).

Variables:

T/K = 293–253

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (complier)		water-rich phase (complier)		hydrocarbon-rich phase		water-rich phase	
20	293.2	0.0000	0.9976	0.0000	0.0001	0.0000	0.9995	0.0000	0.0005
		0.0209	0.9751	0.0767	0.0005	0.0106	0.9886	0.1750	0.0022
		0.0485	0.9441	0.2067	0.0011	0.0250	0.9735	0.3986	0.0041
		0.0797	0.9058	0.2253	0.0047	0.0420	0.9550	0.4205	0.0175
		0.1066	0.8790	0.2546	0.0084	0.0570	0.9400	0.4550	0.0300
		0.1866	0.7907	0.3533	0.0225	0.1050	0.8900	0.5500	0.0700
		0.2548	0.6822	0.4629	0.0778	0.1550	0.8300	0.5800	0.1950
		0.3769	0.5097	0.5027	0.1966	0.2616	0.7076	0.4960	0.3880
		0.4643	0.3570	0.4643	0.3570	0.3720	0.5720	0.3720	0.5720[a]
80.0	353.2	0.0600	0.9152	0.0442	0.0007	0.0316	0.9633	0.1055	0.0034[b]
79.0	352.2	0.0650	0.9098	0.0510	0.0008	0.0343	0.9605	0.1205	0.0037[b]
78.0	351.2	0.0700	0.9001	0.0634	0.0009	0.0372	0.9566	0.1471	0.0042[b]
77.0	350.2	0.0869	0.8780	0.0858	0.0012	0.0468	0.9458	0.1927	0.0054[b]
76.0	349.2	0.1101	0.8480	0.1201	0.0030	0.0604	0.9306	0.2560	0.0128[b]
75.0	348.2	0.1366	0.8020	0.2122	0.0158	0.0774	0.9090	0.3888	0.0580[b]
74.5	347.7	0.2801	0.6000	0.3302	0.0660	0.1834	0.7859	0.4728	0.1891[b]
74.4	347.6	0.3910	0.3401	0.4146	0.1659	0.3324	0.5782	0.4554	0.3644[b]
74.3	347.5	0.4031	0.2276	0.4031	0.2276	0.4020	0.4540	0.4020	0.4540[a,b,c]

[a] Critical solubility point.
[b] Temperatures are the boiling temperatures of the two-phase mixtures.
[c] Boiling temperature estimated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

The method of description of concentration of phases in equilibrium was the same as reported in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified; properties were in agreement with literature data.
(2) source not specified; properties were in agreement with literature data.
(3) Not specified.

Estimated Error:

Not reported.

References:

[1] A S. Mozzhukhin, L. A. Serafimov, and V. A. Mitropolskaya, Zh. Fiz. Khim. **41**, 1687 (1967).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

F. R. Bevia, D. P. Rico, and V. G. Yagues, Fluid Phase Equilib. **23**, 269–92 (1985).

Variables:

T/K = 298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.0878	0.0022	0.196	0.010
		0.2028	0.0034	0.390	0.013
		0.3608	0.0296	0.548	0.090
		0.4245	0.0666	0.561	0.176
		0.4623	0.1221	0.532	0.281
		0.4646	0.2344	0.442	0.446
		0.4195	0.3584	0.343	0.586
		0.3659	0.4608	0.270	0.680
		0.2867	0.5963	0.188	0.782
		0.1721	0.7830	0.098	0.892

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The quaternary system ethanol–toluene–water–chloroform was investigated. Mixtures of known composition representing the chosen ratios of components were vigorously stirred for at least 2 h and then allowed to separate. The refractive indexes of both phases were measured in a thermostated ERMA Abbe refractometer and the results were plotted as function of ethanol concentration. Solubility in the ternary system was calculated from these plots.

Source and Purity of Materials:

(1) Merck, analytical reagent grade; volatile impurities <0.1 mass % by glc.
(2) Merck, analytical reagent grade; volatile impurities <0.1 mass % by glc.
(3) not specified.

Estimated Error:

temp. ±0.1 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Methylbenzene (toluene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

K. Ricna, J. Matous, J. P. Novak, and V. Kubicek, Collect. Czech. Chem. Commun. **54**, 581–5 (1989).

Variables:

T/K=278

Compiled By:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
5.0	278.15	0.8620	0.0356	0.8857	0.0732
		0.7072	0.0587	0.7719	0.1281
		0.5725	0.1045	0.6306	0.2302
		0.3597	0.1978	0.3875	0.4261
		0.2220	0.2780	0.2280	0.5711
		0.0928	0.4151	0.0832	0.7443
		0.0213	0.4251	0.0196	0.7814

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
5.0	278.15	0.0000	0.9938	0.9980	0.0013	0.0000	0.9988	0.9971	0.0026
		0.0000	0.9783	0.9921	0.0052	0.0000	0.9957	0.9886	0.0104
		0.0000	0.9763	0.9919	0.0051	0.0000	0.9953	0.9887	0.0102
		0.0000	0.9447	0.9888	0.0036	0.0000	0.9887	0.9898	0.0072
		0.0000	0.8855	0.9744	0.0050	0.0000	0.9753	0.9818	0.0101
		0.0000	0.8197	0.9546	0.0053	0.0000	0.9588	0.9732	0.0108
		0.0061	0.7283	0.9080	0.0168	0.0039	0.9298	0.9351	0.0346
		0.0255	0.6037	0.8516	0.0235	0.0185	0.8763	0.8988	0.0496
		0.0361	0.5554	0.8331	0.0310	0.0276	0.8501	0.8786	0.0654
		0.0442	0.5171	0.8091	0.0418	0.0354	0.8274	0.8508	0.0879
		0.0655	0.4727	0.7895	0.0369	0.0550	0.7935	0.8478	0.0793
		0.0996	0.3951	0.7435	0.0512	0.0916	0.7267	0.8028	0.1106
25.0	298.15	0.0000	0.9930	0.9973	0.0014	0.0000	0.9986	0.9967	0.0028
		0.0000	0.9745	0.9932	0.0020	0.0000	0.9949	0.9941	0.0040
		0.0000	0.9364	0.9770	0.0072	0.0000	0.9869	0.9794	0.0144
		0.0072	0.8082	0.9062	0.0232	0.0042	0.9532	0.9245	0.0473
		0.0176	0.6710	0.8236	0.0332	0.0119	0.9059	0.8706	0.0702
		0.0170	0.6530	0.8349	0.0295	0.0117	0.8994	0.8817	0.0623
		0.0305	0.6093	0.7857	0.0460	0.0219	0.8767	0.8327	0.0975
		0.0571	0.5171	0.7374	0.0586	0.0454	0.8222	0.7892	0.1254
		0.0947	0.4518	0.6349	0.0963	0.0806	0.7686	0.6808	0.2065
		0.1172	0.4227	0.6200	0.1000	0.1026	0.7399	0.6670	0.2152
		0.1265	0.4009	0.6194	0.0998	0.1136	0.7203	0.6669	0.2149
50.0	323.15	0.0000	0.9928	0.9960	0.0013	0.0000	0.9986	0.9963	0.0026
		0.0000	0.9908	0.9927	0.0038	0.0000	0.9982	0.9910	0.0076
		0.0000	0.9674	0.9803	0.0058	0.0000	0.9935	0.9829	0.0116
		0.0000	0.9534	0.9757	0.0027	0.0000	0.9905	0.9860	0.0055
		0.0030	0.9447	0.9672	0.0073	0.0016	0.9877	0.9752	0.0147
		0.0047	0.8252	0.8669	0.0275	0.0027	0.9586	0.9000	0.0571
		0.0068	0.7929	0.8333	0.0439	0.0041	0.9491	0.8598	0.0906
		0.0081	0.7481	0.7961	0.0488	0.0051	0.9353	0.8342	0.1023
		0.0331	0.6856	0.7719	0.0552	0.0219	0.9055	0.8126	0.1162
		0.0306	0.6403	0.7294	0.0655	0.0213	0.8894	0.7755	0.1393
		0.0428	0.6082	0.6888	0.0764	0.0307	0.8716	0.7379	0.1637
		0.1021	0.5045	0.5390	0.1570	0.0807	0.7977	0.5546	0.3231
		0.1256	0.4592	0.4553	0.2033	0.1041	0.7613	0.4574	0.4085
		0.1603	0.4146	0.3320	0.2726	0.1387	0.7175	0.3218	0.5284

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used for solubility measurements. Water was added from a calibrated hypodermic syringe (controlled by a micrometer screw) to a binary ethanol–toluene mixture of known mass and composition until persistent turbidity was observed. The direct analytical method was used for liquid–liquid equilibrium measurements. A mixture was stirred vigorously for 2–3 h in a thermostated cell, [1] and after phase separation samples were taken for analysis. A small amount of tetrahydrofuran was added as an internal standard and homogenization agent in glc analysis. Calibration standards were analyzed separately for each phase prior to each sample analysis by glc. Conditions of the glc analysis were: glass column (2.5 mm i.d., 1.5 m), Poropak Q, 200 °C, carrier gas H_2, thermal conductivity detector.

Source and Purity of Materials:

(1) source not specified ''extra fine;'' distilled with benzene; 0.1% H_2O by the Karl Fischer method; $\rho(25\ °C) = 0.784\ 98$ g cm^{-3}, $n(25\ °C,D) = 1.3605$.
(2) Lachema Neratovice, A. R. grade; shaken five times with H_2SO_4 conc., three times with H_2O, then with NaOH, dried with Na, distilled; $\rho(25\ °C) = 0.861\ 24$ g/cm^3, $n(25\ °C,D) = 1.4939$.
(3) doubly distilled.

Estimated Error:

temp. ±0.05 K.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K = 298

Complied by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.174	0.001	0.349	0.004
		0.242	0.003	0.445	0.011
		0.319	0.014	0.525	0.046
		0.404	0.041	0.575	0.117
		0.424	0.053	0.577	0.144
		0.460	0.099	0.554	0.238
		0.472	0.159	0.505	0.340
		0.456	0.228	0.440	0.440
		0.430	0.323	0.367	0.551
		0.378	0.441	0.284	0.663
		0.296	0.591	0.194	0.777
		0.174	0.785	0.099	0.892
		0.094	0.889	0.050	0.946
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K(compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.341	0.510	0.470	0.170	0.240	0.719	0.494	0.358
		0.285	0.610	0.466	0.112	0.184	0.789	0.545	0.262
		0.230	0.697	0.445	0.070	0.139	0.844	0.572	0.185
		0.178	0.778	0.410	0.042	0.102	0.889	0.579	0.119
		0.090	0.890	0.315	0.012	0.048	0.940	0.523	0.040

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; $d = 0.78524$, $n = 1.3594$.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wooten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18,** 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Methylcyclohexane (hexahydrotoluene); C_7H_{14}; [108-87-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130–2 (1945).

Variables:

T/K=228–298

Compiled by:

A. Skrzecz

4.7. Ethanol + Water + Methylcyclohexane

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	x_2 (compiler)
−45.0	228.2	0.8952	0.0527	0.7251	0.2327
		0.8320	0.1470	0.5030	0.4843
		0.6471	0.3429	0.2562	0.7399
0.0	273.2	0.8580	0.0505	0.7005	0.2248
		0.8091	0.1429	0.4946	0.4761
		0.6366	0.3373	0.2545	0.7351
25.0	298.2	0.8349	0.0492	0.6850	0.2198
		0.7922	0.1399	0.4882	0.4700
		0.6275	0.3325	0.2530	0.7308

Comments and Additional Data

Water tolerance (S) was described with probable error $< 0.5\%$ at the range −45–25 °C by the equation: $\log(S)=a-b/(T/\mathrm{K})$. The parameters ($a$,$b$) were determined from plots. Water tolerance was defined as: $S=H_2O$ % by volume·(100-Hydrocarbon % by volume in the blend)/100.

vol % hydrocarbon	a	b
75	2.058	587.6
50	2.210	504.9
25	2.047	347.3

Auxiliary Information

Method/Apparatus/Procedure:

A glass tube with stirrer containing the ternary mixture was immersed in a bath, the temperature of which could be varied. Mixtures were prepared directly in the tube, by special pipettes at 15.5 °C. Precautions to exclude moisture and to prevent evaporation were observed. No correction was made for the slight expansion in volume when alcohol was mixed with hydrocarbon. In the paper the experimental results were expressed as the water tolerance of the alcohol–hydrocarbon blend. For practical purposes water tolerance was defined as the volume percent of water which can be added before separation occurs.

Source and Purity of Materials:

(1) source not specified; anhydrous ethanol.
(2) source not specified; b.p.=99.85–100 °C.
(3) not specified.

Estimated Error:

temp. within about 0.3 °C (duplicate determinations), composition <0.2% relative of volume fraction.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) 1-Heptene; C_7H_{14}; [592-76-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, B. C. Bricknell, I. D. Sewry, and S. E. Radloff, J. Chem. Eng. Data **39**, 320–3 (1994).

Variables:

T/K=298

Compiled by:

A. Skrzecz

4.8. Ethanol + Water + 1-Heptene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	1.000	0.000	1.000
		0.202	0.770	0.109	0.885
		0.361	0.579	0.223	0.762
		0.455	0.457	0.311	0.666
		0.538	0.342	0.409	0.555
		0.596	0.248	0.503	0.446
		0.628	0.171	0.586	0.340
		0.637	0.113	0.653	0.247
		0.611	0.063	0.700	0.154
		0.513	0.022	0.692	0.063
		0.412	0.013	0.620	0.042
		0.300	0.010	0.507	0.036
		0.239	0.005	0.438	0.020
		0.047	0.001	0.112	0.005
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x_1	x_2	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.365	0.578	0.595	0.246	0.225	0.761	0.504	0.444
		0.330	0.620	0.627	0.175	0.197	0.791	0.582	0.346
		0.262	0.700	0.639	0.121	0.148	0.843	0.645	0.260
		0.228	0.743	0.555	0.033	0.125	0.869	0.706	0.089
		0.193	0.783	0.442	0.017	0.103	0.892	0.641	0.053
		0.099	0.890	0.239	0.005	0.049	0.948	0.438	0.020

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods have been described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) Aldrich; distilled; purity >99.8 mole % by glc, $\rho = 0.692\ 65$ g cm^{-3}.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water (hydrogen oxide); H_2O; [7732-18-5]

Evaluted by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.03)

4.9. Ethanol + Water + Heptane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of ethanol between phases (distr.) for the system ethanol–heptane–water is given in Table 28.

TABLE 28. Summary of experimental data for the system ethanol–heptane–water

Author(s)	T/K	Type of data[a]	Ref.
Bonner, 1909	273	sat. (9)	1
Schweppe and Lorah, 1954	303	sat. (24), distr. (7)	2
Vorobeva and Karapetyants, 1966	298	sat. (15), eq.(9)	3
Letcher *et al.*, 1986	298	sat. (8), eq.(3)	4

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system ethanol–heptane–water forms a large miscibility gap of type 1 covering the majority of the concentration triangle. The system was investigated by four groups over the temperature range 273–303 K; the saturation data are consistent with one another. Only the heptane–water binary system forms a miscibility gap. The data of this system were compiled and critically evaluated in a previously published SDS volume,[5] the recommended values at 298 K are: $x_2'' = 4.3 \cdot 10^{-7}$ and $x_3' = 5.6 \cdot 10^{-4}$. The data reported by Schweppe and Lorah,[2] at 303 K, and Vorobeva and Karapetyants,[3] at 298 K, include solubility of the binary system heptane–water; $x_2'' = 0.0003$ and $x_3' < 0.005$, respectively. These values are less precise and do not agree with the recommended data reported in Ref. 5. All experimental solubility and equilibrium data reported at 298 K in Refs. 3 and 4, were described by the equation:

$$x_1 = 1.1136 + 0.1319 \ln(x_2) - 1.2083 x_2 + 0.0932 x_2^2.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0087. The selected points on the saturation curve, calculated by the above equation together with the ''best'' values of Ref. 5 are presented in Table 29 as in Fig. 1 as solid line.

TABLE 29. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 000 43 Ref. 5	0.4242	0.5200
0.5735	0.0200	0.4070	0.5400
0.6408	0.0400	0.3897	0.5600
0.6703	0.0600	0.3723	0.5800
0.6844	0.0800	0.3548	0.6000
0.6900	0.1000	0.3372	0.6200
0.6903	0.1200	0.3196	0.6400
0.6869	0.1400	0.3019	0.6600
0.6809	0.1600	0.2842	0.6800
0.6729	0.1800	0.2664	0.7000
0.6634	0.2000	0.2486	0.7200
0.6526	0.2200	0.2308	0.7400
0.6407	0.2400	0.2129	0.7600
0.6281	0.2600	0.1951	0.7800
0.6147	0.2800	0.1772	0.8000
0.6007	0.3000	0.1593	0.8200
0.5862	0.3200	0.1414	0.8400
0.5713	0.3400	0.1235	0.8600
0.5559	0.3600	0.1056	0.8800
0.5403	0.3800	0.0877	0.9000
0.5243	0.4000	0.0699	0.9200
0.5081	0.4200	0.0520	0.9400
0.4917	0.4400	0.0341	0.9600
0.4751	0.4600	0.0163	0.9800
0.4583	0.4800	0.0000	0.999 44 Ref. 5
0.4413	0.5000		

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system ethanol–heptane–water were reported in Refs. 3 and 4 at 298.2 K. The reported equilibrium data sets are not consistent with one another, although they are consistent within each data set. The data for phases in equilibrium differ very much from one another; they are treated as doubtful. Part of experimental tie lines from both discussed references are crossing one another and therefore they are rejected and not reported in Fig. 15. These tie lines cover the region of high heptane concentration (>0.79 mole fraction) in the heptane-rich phase.

The plait point at 298.2 K reported in Ref. 3 is $x_1 = 0.517$ and $x_2 = 0.409$.

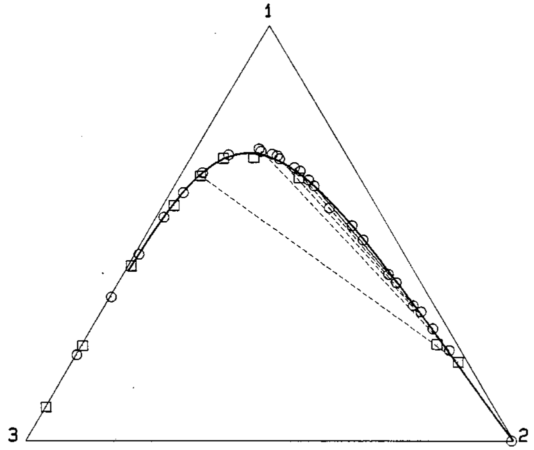

FIG. 15. Phase diagram of the system ethanol (1)—heptane (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 3, □—experimental data, Ref. 4, dashed lines—experimental tie lines, Refs. 3 and 4.

References:

[1] W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).

[2] J. L. Schweppe and J. R. Lorah, Ind. Eng. Chem. **46**, 2391 (1954).

[3] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).

[4] T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

[5] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910).

Variables:
T/K=273

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K(compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (complier)	w_2 (complier)
0.0	273.2	0.5662	0.3557	0.4131	0.5646
		0.7044	0.1695	0.6276	0.3285
		0.7289	0.1126	0.7037	0.2364
		0.7145	0.0736	0.7462	0.1673
		0.7030	0.0656	0.7509	0.1524
		0.6640	0.0438	0.7601	0.1092
		0.6086	0.0250	0.7549	0.0674
		0.5797	0.0176	0.7475	0.0495
		0.4939	0.0092	0.6974	0.0281

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogenous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:
(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated error:
accuracy of weighing 0.0001 g.

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2)Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
J. L. Schweppe and J.R. Lorah, Ind. Eng. Chem. **46**, 2391–2 (1954).

Variables:
T/K=303

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
30.00	303.15	0.2061	0.7890	0.1071	0.8919
		0.3650	0.6296	0.2102	0.7886
		0.4437	0.5078	0.2831	0.7048
		0.5318	0.4133	0.3662	0.6190
		0.5996	0.3124	0.4565	0.5173
		0.6226	0.2892	0.4841	0.4891
		0.6865	0.1889	0.5990	0.3585
		0.6687	0.2222	0.5597	0.4046
		0.6298	0.2674	0.5032	0.4647
		0.6997	0.1458	0.6495	0.2944
		0.7090	0.1137	0.6913	0.2411
		0.6963	0.0784	0.7292	0.1785
		0.6912	0.0636	0.7469	0.1495
		0.6477	0.0398	0.7563	0.1010
		0.4764	0.0073	0.6862	0.0230
		0.4957	0.0073	0.7021	0.0226
		0.5784	0.0135	0.7537	0.0384
		0.6367	0.0253	0.7727	0.0669
		0.6587	0.0394	0.7638	0.0993
		0.2808	0.0005	0.4988	0.0021
		0.1155	0.0002	0.2502	0.0009
		0.3727	0.0026	0.5986	0.0090
		0.0000	0.0003	0.0000	0.0016
		0.2738	0.0005	0.4901	0.0019

Distribution of ethanol in ethanol–heptane–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_1'' water-rich phase
30.00	303.15	0.029	0.106
		0.032	0.290
		0.050	0.392
		0.050	0.460
		—	0.624
		0.055	0.752
		0.145	0.663

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Third component (hexane or water) was added to the binary alcohol solutions, respectively, held in a temperature controlled bath until a cloud point was observed. The solutions were prepared by weight, using an analytical balance. Density and refractive index measurements were made for the mixture and then plotted separately for each component. Then tie lines were determined by analytical method. The two-phase mixtures were placed in a thermostated bath and agitated periodically. After phase separation, densities of both phases were measured and concentrations were read from the plots. Phase equilibrium data were reported in incomplete form; only distribution of ethanol between water and heptane was reported.

Source and Purity of Materials:

(1) U.S. Industrial Chemicals, Inc., U.S.P., 200-proof; $n(30\ °C)=1.3579$; used as received.
(2) Philips Petroleum Co., pure grade; purity>99 mole %, $n(30\ °C)=1.3835$.
(3) distilled.

Estimated Error:

temp. ±0.03 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018–23 (1966). [Eng. transl. Russ. J. Phys. Chem. **40**, 1619–22 (1966)].

Variables:

$T/K=298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9945	0.000	0.999
		0.3108	0.6535	0.178	0.814
		0.4828	0.4488	0.325	0.657
		0.5591	0.3415	0.417	0.554
		0.6474	0.2381	0.535	0.428
		0.6843	0.1730	0.613	0.337
		0.6877	0.1609	0.627	0.319
		0.7009	0.1279	0.670	0.266
		0.6868	0.0730	0.731	0.169
		0.6432	0.0413	0.751	0.105
		0.5959	0.0257	0.745	0.070
		0.5372	0.0151	0.721	0.044
		0.4486	0.0081	0.661	0.026
		0.3467	0.0022	0.572	0.008
		0.2070	0.0010	0.399	0.004

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/°C$	T/K (compiler)	hyrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.000	1.000	0.365	0.003	<0.001	1.000	0.591	0.009
		0.030	0.970	0.492	0.008	0.014	0.986	0.697	0.026
		0.128	0.857	0.692	0.086	0.064	0.933	0.716	0.194
		0.218	0.758	0.695	0.135	0.116	0.879	0.659	0.278
		0.270	0.698	0.677	0.181	0.150	0.843	0.601	0.350
		0.326	0.630	0.656	0.222	0.190	0.800	0.553	0.407
		0.381	0.568	0.626	0.266	0.233	0.755	0.502	0.464
		0.401	0.542	0.612	0.284	0.250	0.736	0.482	0.486
		0.517	0.409	0.517	0.409	0.360	0.620	0.360	0.620

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, Ref. 1, was used to determine solubility of the mixtures. The third component was added to the binary homogenous mixture until cloudiness was first observed. Density of the saturated mixtures was measured; these results were graphed. To obtain equilibrium, ternary mixtures were stirred in a thermostated vessel for several hours. After phase separation, the density of each phase was measured and composition was determined from the graphs prepared earlier. Concentration at the critical point was found by method described in Ref. 2. Water included in ethanol was taken into account in all measurements.

Source and Purity of Materials:

(1) source not specified, ''rectificate grade:'' distilled; water concentration was determined by the Karl Fischer method.
(2) source not specified; b.p. = 98.4 °C, $n(20\ °\text{C,D}) = 1.3877$.
(3) not specified.

Estimated Error:

solubility ±0.001 mass fraction.

References:

[1] W. D. Bancroft, Phys. Rev. **3**, 21 (1896).
[2] E. N. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Heptane (n-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:

$T/\text{K} = 298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°\text{C}$ (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.082	0.000	0.186	0.000
		0.229	0.002	0.429	0.008
		0.421	0.006	0.640	0.020
		0.565	0.022	0.730	0.062
		0.678	0.067	0.734	0.158
		0.680	0.128	0.658	0.269
		0.631	0.244	0.521	0.438
		0.232	0.726	0.127	0.864

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1''	w_2'	w_1''	w_2''
$t/°\text{C}$ (compiler)	T/K	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25	298.2	0.190	0.790	0.636	0.041	0.099	0.897	0.747	0.105
		0.110	0.875	0.418	0.006	0.054	0.943	0.637	0.020
		0.078	0.912	0.138	0.002	0.038	0.960	0.288	0.009

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) NCP, South Africa, absolute grade; dried with magnesium metal activated with iodine, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1] S . W. Briggs and E. W. Commings, Ind. Eng. Chem. **35**, 411 (1943).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *m*-Xylene (1,3-dimethylbenzene, 1,3-xylene); C_8H_{10}; [108-38-3]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.04)

4.10. Ethanol + Water + *m*-Xylene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system ethanol–*m*-xylene–water is given in Table 30.

TABLE 30. Summary of experimental data for the system ethanol–*m*-xylene–water

Author(s)	T/K	Type of data[a]	Ref.
Bonner, 1909	273	sat. (10)	1
Holt and Bell, 1914	273–373	sat.(43)	2
Mochalov, 1937	273, 323	eq.(12)	3
Leikola, 1940	293	sat. (6)	4
Mondain-Monval and Quiquerez, 1940	298	sat. (22), eq. (8)	5
Nam *et al.*, 1972	298	sat. (16), eq. (10)	6

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system ethanol–*m*-xylene–water forms a miscibility gap of type 1. This critical evaluation is based on the original papers with the exception of data of Mochalov[3] and Leikola[4] which were taken from the handbooks of Seidel and Linke[7] and Kafarov,[8] respectively; these data sets were also taken into account during evaluation but are not reported as compilation sheets because they do not contribute further to knowledge of the system. Data of Holt and Bell[2] measured over a wide temperature range, show a decreasing miscibility gap with increasing temperature which is in agreement with the general expectation. The points $x_1=0.4706$ at 336.2 K and $x_1=0.3956$ at 373.2 K are incompatible with other data and presumably contain experimental errors. Data of Leikola[4] for 293 K are close to the data for 298.2 K, with the exception of one experimental point $x_1=0.561$, $x_2=0.243$, which presumably contains an experimental error. Other solubility data are consistent within each data set, at the same temperature as well as with one another. Nam *et al.*,[6] checked their experiments in two ways: repetition of experiment with another mixture and by reappearance of turbidity by lowering the temperature; so these data are considered more reliable. Equilibrium compositions of both phases, reported in Ref. 6, are consistent with saturation measurements. Only one binary system, *m*-xylene–water, forms a miscibility gap. This system was compiled and critically evaluated in a previously published SDS vol. 38, Ref. 9. These recommended values are: $x_2'=0.000\ 0344$ and $x_2''=0.9989$ at 273 K; $x_2'=0.000\ 029$ and $x_2''=0.9978$ at 293 K and $x_2'=0.000\ 027$ and $x_2''=0.9974$ at 298 K. All experimental data are treated as tentative. Data reported at 298.2 K by Mondain-Monval and Quiquerez[5] and Nam *et al.*,[6] $x_2<0.96$ (water-rich and hydrocarbon-rich branches were treated together), were used to construct the fitting equation:

$$x_1=0.765\ 79+0.087\ 29\ln(x_2)-0.495\ 55x_2-0.284\ 48x_2^2.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0164. Selected points on the saturation curve, calculated by this equation together with the recommended values of Ref. 9 are presented in Table 31 and in Fig. 16 as the solid line. Experimental points at 298.2 K are also shown.

TABLE 31. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 027 Ref. 9	0.3983	0.4800
0.1623	0.0010	0.3864	0.5000
0.3588	0.0100	0.3741	0.5200
0.4143	0.0200	0.3615	0.5400
0.4645	0.0400	0.3485	0.5600
0.4894	0.0600	0.3351	0.5800
0.5038	0.0800	0.3215	0.6000
0.5124	0.1000	0.3075	0.6200
0.5171	0.1200	0.2932	0.6400
0.5192	0.1400	0.2785	0.6600
0.5192	0.1600	0.2636	0.6800
0.5177	0.1800	0.2484	0.7000
0.5148	0.2000	0.2328	0.7200
0.5108	0.2200	0.2170	0.7400
0.5059	0.2400	0.2009	0.7600
0.5001	0.2600	0.1845	0.7800
0.4936	0.2800	0.1678	0.8000
0.4864	0.3000	0.1508	0.8200
0.4789	0.3200	0.1336	0.8400
0.4702	0.3400	0.1160	0.8600
0.4613	0.3600	0.0982	0.8800
0.4519	0.3800	0.0802	0.9000
0.4421	0.4000	0.0618	0.9200
0.4318	0.4200	0.0432	0.9400
0.4210	0.4400	0.0243	0.9600
0.4099	0.4600	0.0000	0.9974 Ref. 9

Phases in equilibrium

The equilibrium data for the ternary system ethanol–*m*-xylene–water were reported in the papers of Mochalov,[3] Mondain-Monval and Quiquerez,[5] and Nam *et al.*[6] At 298.2 K data of Mondain-Monval and Quiquerez[5] covered the region closer to the plait point, while data of Nam *et al.*[6] covered the region from low methanol concentrations to the equilibrium point ($x_1=0.412$, $x_2=0.024$ in water-rich phase). The results are consistent within each data set but there is significant disagreement between the first tie line of Ref. 5 ($x_1''=0.261$ and $x=0.002$) and the tie lines reported by Nam *et al.*[6] Other reported tie lines are consistent. Systematic changes in the partition coefficient of ethanol are observed with temperature. Characteristic points on the binodal curve, plait point and maximum ethanol concentration, reported or estimated, are presented at selected temperatures in Table 32. The errors of maximum ethanol concentration point estimated by the evaluator are 0.01 and 0.02 mole fraction of ethanol and *m*-xylene, respectively.

TABLE 32. Characteristic points on binodal curve of the system ethanol–*m*-xylene–water

	Max. C_2H_5OH concentration			Plait points		
T/K	x_1	x_2	Ref.	x_1	x_2	Ref.
273.2	0.59	0.19	1	0.549	0.329	3
298.2	0.53	0.15	5	0.470	0.324	5
298.2	0.53	0.13	6	—	—	
314.2	0.51	0.15	2	—	—	
323.2	—	—		0.492	0.274	3
336.2	0.46	0.16	2	—	—	

The experimental data for phase equilibria at 298.2 K are considered tentative and are presented in the Fig. 16.

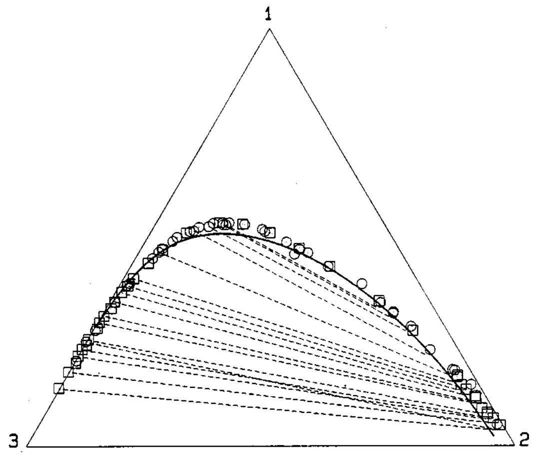

FIG. 16. Phase diagram of the system ethanol (1)—*m*-xylene (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 5, □—experimental data, Ref. 6, dashed lines—experimental tie lines, Refs. 5 and 6.

References:

[1] W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).

[2] A. Holt and N. M. Bell, J. Chem. Soc. **105**, 633 (1914).

[3] K. I. Mochalov, Izv. Biol. Nauchno-Issled. Inst. Molotov. Gos. Univ. **11**, 25 (1937).

[4] E. Leikola, Suomen Kemistil. B **13**, 13 (1940).

[5] P. I. Mondain-Monval and J. Quiquerez, Bull. Soc. Chim. Fr. Mem. **7**, 240 (1940).

[6] S. Nam, T. Hayakawa, and S. Fujita, J. Chem. Eng. Jpn. **5**, 327 (1972).

[7] A. Seidel and W. F. Linke, *Solubilities of Inorganic and Organic Compounds*, Supplement to the Third Edition, Am. Chem. Soc., D (Ban Nostrand Co., New York, 1952).

[8] V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskva, 1963).

[9] D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *m*-Xylene (1,3-dimethylbenzene, 1,3-xylene); C_8H_{10}; [108-38-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910)

Variables:

T/K=273

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
0.0	273.2	0.4350	0.4704	0.2795	0.6967
		0.5548	0.2714	0.4444	0.5011
		0.5912	0.1911	0.5294	0.3944
		0.6028	0.1170	0.6139	0.2745
		0.5772	0.0835	0.6396	0.2133
		0.5387	0.0490	0.6627	0.1390
		0.5036	0.0302	0.6667	0.0920
		0.4684	0.0223	0.6516	0.0714
		0.3953	0.0114	0.6047	0.0403
		0.3177	0.0027	0.5387	0.0106

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogeneous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated Error:

accuracy of weighing 0.0001 g.

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *m*-Xylene (1,3-dimethylbenzene, 1,3-xylene); C_8H_{10}; [108-38-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
A. Holt and N. M. Bell, J. Chem. Soc. **105**, 633–9 (1914).

Variables:
T/K=273–373

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
0	273.2	0.4112	0.4918	0.2598	0.7162
		0.5335	0.3189	0.4023	0.5542
		0.5827	0.2323	0.4895	0.4497
		0.5961	0.1783	0.5443	0.3752
		0.5907	0.1446	0.5749	0.3243
		0.6002	0.1196	0.6091	0.2797
		0.5843	0.0873	0.6393	0.2201
		0.5522	0.0600	0.6557	0.1642
		0.5271	0.0450	0.6604	0.1299
		0.5143	0.0362	0.6649	0.1079
19	292.2	0.4043	0.4836	0.2587	0.7132
		0.5069	0.3031	0.3961	0.5458
		0.5344	0.2131	0.4753	0.4368
		0.5471	0.1636	0.5275	0.3635
		0.5637	0.1318	0.5714	0.3079
		0.5452	0.1087	0.5856	0.2691
		0.5398	0.0922	0.6023	0.2371
		0.5200	0.0691	0.6191	0.1896
		0.4731	0.0404	0.6254	0.1231
		0.4289	0.0223	0.6172	0.0740
41	314.2	0.3853	0.4608	0.2556	0.7045
		0.4719	0.2822	0.3873	0.5338
		0.4963	0.1979	0.4630	0.4255
		0.5075	0.1517	0.5124	0.3530
		0.5075	0.1214	0.5443	0.3001
		0.5007	0.0998	0.5645	0.2593
		0.4661	0.0557	0.5964	0.1643
		0.4437	0.0442	0.5949	0.1366
		0.4122	0.0336	0.5836	0.1096
		0.4035	0.0268	0.5864	0.0898
63	336.2	0.3708	0.4435	0.2530	0.6974
		0.4167	0.3322	0.3254	0.5979
		0.4706	0.2814	0.3870	0.5333
		0.4522	0.2163	0.4186	0.4614
		0.4606	0.1836	0.4503	0.4137
		0.4644	0.1587	0.4751	0.3741
		0.4564	0.1248	0.5028	0.3168
		0.4566	0.0993	0.5315	0.2664
		0.4495	0.0766	0.5540	0.2176
		0.4035	0.0419	0.5628	0.1347
100	373.2	0.3956	0.1881	0.3988	0.4370
		0.3824	0.0759	0.4972	0.2274
		0.4097	0.0375	0.5752	0.1213

Distribution of *m*-xylene in ethanol—*m*-xylene—water system

t/°C	T/K (compiler)	x_2' hydrocarbon-rich phase (compiler)	x_2'' water-rich phase (compiler)
0	273.2	0.8018	0.0093
0	273.2	0.6995	0.0229
19	292.2	0.8212	0.0105
19	292.2	0.5840	0.0527

Auxiliary Information

Method/Apparatus/Procedure:

To a known volume of *m*-xylene small portions of alcohol were added. After each addition of alcohol, water was added until a distinct milkiness was observed. The mixture was kept at constant temperature and was shaken repeatedly.

Source and Purity of Materials:

(1) source not specified; ''absolute'' ethyl alcohol; used as received.
(2) source not specified; ''nearly pure'' *m*-xylene; used as received.
(3) distilled.

Estimated Error:

Not reported.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *m*-Xylene (1,3-dimethylbenzene, 1,3-xylene); C_8H_{10}; [108-38-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. Mondain-Monval and J. Quiquerez, Bull. Soc. Chim. Fr. Mem. **7**, 240–53 (1940).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.00	298.15	0.2039	0.0006	0.3948	0.0029
	298.15	0.2763	0.0036	0.4880	0.0145
	298.15	0.3433	0.0105	0.5536	0.0389
	298.15	0.3887	0.0176	0.5876	0.0614
	298.15	0.4485	0.0344	0.6144	0.1086
	298.15	0.4717	0.0421	0.6216	0.1279
	298.15	0.4992	0.0592	0.6175	0.1689
	298.15	0.4895	0.0553	0.6158	0.1602
	298.15	0.5132	0.0783	0.6014	0.2114
	298.15	0.5238	0.0917	0.5915	0.2387
	298.15	0.5328	0.1163	0.5680	0.2857
	298.15	0.5345	0.1343	0.5490	0.3180
	298.15	0.5344	0.1479	0.5347	0.3410
	298.15	0.5304	0.1818	0.4995	0.3945
	298.15	0.5185	0.2237	0.4569	0.4543
	298.15	0.5133	0.2312	0.4479	0.4649
	298.15	0.4877	0.2887	0.3932	0.5363
	298.15	0.4618	0.3456	0.3463	0.5972
	298.15	0.4287	0.4037	0.3009	0.6531
	298.15	0.3870	0.4940	0.2462	0.7242
	298.15	0.3168	0.5931	0.1843	0.7952
	298.15	0.1803	0.7874	0.0898	0.9039

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.051	0.938	0.261	0.002	0.023	0.975	0.470	0.010
	298.15	0.146	0.838	0.395	0.019	0.070	0.927	0.591	0.066
	298.15	0.182	0.782	0.475	0.044	0.091	0.902	0.621	0.133
	298.15	0.229	0.713	0.526	0.090	0.121	0.867	0.595	0.235
	298.15	0.285	0.646	0.537	0.115	0.158	0.827	0.573	0.282
	298.15	0.320	0.592	0.541	0.142	0.186	0.794	0.545	0.330
	298.15	0.342	0.555	0.541	0.148	0.206	0.770	0.539	0.340
	298.15	0.470	0.324	0.470	0.324	0.362	0.576	0.362	0.576[a]

[a]Plait point.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. 100 mL of ternary mixture, prepared by weight, was placed in thermostat, agitated many times and then leave for several hours to separate. The density and refractive index of each phase was measured. Inversion of density was observed.

Source and Purity of Materials:

(1) source not specified; d(25 °C,4 °C)=0.7853.
(2) source not specified; d(25 °C, 4 °C)=0.8593, b.p. =138.1 °C at 739 Torr.
(3) not specified.

Estimated Error:

temp. ±0.02 °C.

Components:	**Original Measurements:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) *m*-Xylene (1,3-dimethylebenzene, 1,3-xylene); C_8H_{10}; [108-38-3] (3) Water; H_2O; [7732-18-5]	S. Nam, T. Hayakawa, and S. Fujita, J. Chem. Eng. Jpn. **5**, 327–34 (1972).
Variables: T/K=298	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.00	298.15	0.1678	0.8001	0.0829	0.9109
		0.2748	0.6548	0.1517	0.8331
		0.3464	0.5499	0.2094	0.7661
		0.4281	0.4081	0.2988	0.6565
		0.4730	0.3222	0.3651	0.5731
		0.5102	0.2433	0.4371	0.4803
		0.5310	0.1772	0.5040	0.3877
		0.5349	0.1275	0.5567	0.3059
		0.5097	0.0729	0.6061	0.1998
		0.4685	0.0447	0.6150	0.1351
		0.4368	0.0309	0.6100	0.0993
		0.3816	0.0175	0.5809	0.0613
		0.3284	0.0096	0.5388	0.0364
		0.2806	0.0052	0.4907	0.0210
		0.2410	0.0028	0.4437	0.0117
		0.1988	0.0015	0.3861	0.0065

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.049	0.945	0.1506	0.0008	0.022	0.977	0.311	0.004
		0.066	0.923	0.1888	0.0015	0.030	0.968	0.371	0.007
		0.076	0.907	0.2272	0.0021	0.035	0.962	0.426	0.009
		0.080	0.903	0.2430	0.0031	0.037	0.960	0.446	0.013
		0.090	0.888	0.2662	0.0044	0.042	0.954	0.474	0.018
		0.114	0.864	0.3068	0.0069	0.054	0.942	0.519	0.027
		0.118	0.860	0.3221	0.0084	0.056	0.940	0.534	0.032
		0.134	0.834	0.3562	0.0129	0.065	0.929	0.563	0.047
		0.145	0.818	0.3789	0.0164	0.071	0.922	0.580	0.058
		0.164	0.800	0.4118	0.0239	0.081	0.912	0.599	0.080

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine solubility curve. A binary ethanol–xylene mixture of known composition was prepared in a conical flask with silicone stopper to prevent evaporation. The mixture was placed in a thermostated vessel, agitated by a magnetic stirrer and titrated through a needle of the syringe with water until two phases were observed. The result was checked by another ternary mixture, of the same composition as above: (a) titrated with one of the pure components until the turbidity disappeared, (b) by reappearance of turbidity by lowering the temperature about 0.5 °C. The two-phase mixture was placed in a 50 mL glass-stoppered test tube at temperature of 25 °C, shaken vigorously, kept for nearly 2 h in a constant temperature water bath, and after separation each layer was pipetted for sampling. Refractive index and density of each phase were measured and composition was found from the calibration curves constructed during solubility measurements. When mixtures were not separated clearly after several hours, a centrifuge was used to obtain separation.

Source and Purity of Materials:

(1) Wako Pure Chemical Inst. Ltd., guaranteed reagent; $\rho(25\ °C)=785.32$ kg m^{-3}, $n(25\ °C,D)=1.3600$; used as received.
(2) Kishida Chem. Ltd., guaranteed reagent; $\rho(25\ °C)=859.88$ kg m^{-3}, $n(25\ °C,D)=1.4940$; used as received.
(3) ion exchanged, distilled.

Estimated Error:

temp. ±0.02 °C and ±0.1 °C (near plait point).

Components:	**Evaluated by:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) *o*-Xylene (1,2-dimethylbenzene, 1,2-xylene); C_8H_{10}; [95-47-6] (3) Water; H_2O; [7732-18-5]	A. Skrzecz (1995.04)

4.11. Ethanol + Water + *o*-Xylene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system ethanol–*o*-xylene–water is given in Table 33.

TABLE 33. Summary of experimental data for the system ethanol–*o*-xylene–water

Author(s)	T/K	Type of data[a]	Ref.
Bonner, 1909	273	sat. (10)	1
Nam *et al.*, 1972	298	sat. (16), eq. (10)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system ethanol–*o*-xylene–water forms a miscibility gap of type 1. The system was measured at temperatures 273 and 298 K in two references. Only one binary system, *o*-xylene–water, forms a miscibility gap. Binary data were compiled and critically evaluated in a previously published SDS volume.[3] The recommended values of mutual solubility of the *o*-xylene–water system at 298 K are: $x_2'=0.9974$ and $x_2''=0.000\,029\,3$.[3] Binary data were not reported together with the ternary system and data reported in the both references are far from the binary systems. Experimental errors were ±0.05 mass % (estimated by the evaluator) for data reported in Ref. 1 and ±0.1 mass % (estimated by the authors) for data reported in Ref. 2. Experimental data for phases in equilibrium, reported in Ref. 2, were also used to construct the binodal curve. Although the composition of the *o*-xylene-rich phase is outside the saturation measurements and is scattered, the data appear to be consistent within one another. The data reported from both references appear consistent although they were measured at different temperatures. The system shows increasing solubility with temperature. Data at both temperatures are treated as tentative. The data at 298.2 K (Ref. 2) were described by the equation:

$$x_1=0.746\,15+0.086\,71\ln(x_2)-0.437\,11x_2-0.325\,75x_2^2.$$

The least-squares method was used. The standard error of estimate was 0.0127. The model is not valid in the region of high concentration of *o*-xylene ($x_2>0.98$). Compositions on the saturation curve calculated by the equation are presented in Table 34 for selected concentrations of *o*-xylene in the mixture. The results of calculations (solid line) are presented also graphically (Fig. 17) together with all experimental data reported at 298.2 K.

TABLE 34. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 0293 Ref. 3	0.3861	0.5000
0.1468	0.0010	0.3741	0.5200
0.3424	0.0100	0.3617	0.5400
0.3981	0.0200	0.3489	0.5600
0.4490	0.0400	0.3358	0.5800
0.4748	0.0600	0.3223	0.6000
0.4901	0.0800	0.3085	0.6200
0.4995	0.1000	0.2943	0.6400
0.5052	0.1200	0.2797	0.6600
0.5081	0.1400	0.2648	0.6800
0.5090	0.1600	0.2496	0.7000
0.5082	0.1800	0.2341	0.7200
0.5061	0.2000	0.2182	0.7400
0.5029	0.2200	0.2020	0.7600
0.4987	0.2400	0.1855	0.7800
0.4937	0.2600	0.1686	0.8000
0.4878	0.2800	0.1515	0.8200
0.4813	0.3000	0.1340	0.8400
0.4741	0.3200	0.1162	0.8600
0.4663	0.3400	0.0981	0.8800
0.4580	0.3600	0.0797	0.9000
0.4491	0.3800	0.0611	0.9200
0.4397	0.4000	0.0421	0.9400
0.4299	0.4200	0.0228	0.9600
0.4196	0.4400	0.0032	0.9800
0.4088	0.4600	0.0000	0.9974 Ref. 3
0.3976	0.4800		

Phases in equilibrium

For the ternary system ethanol–*o*-xylene–water, phases, in equilibrium were measured only in Ref. 2 at temperature 298.2 K. The tie lines cover the middle area of miscibility gap and are consistent with one another. They are considered tentative. The plait point was not reported. All experimental data reported at 298.2 K, Ref. 2, are presented in Fig. 17.

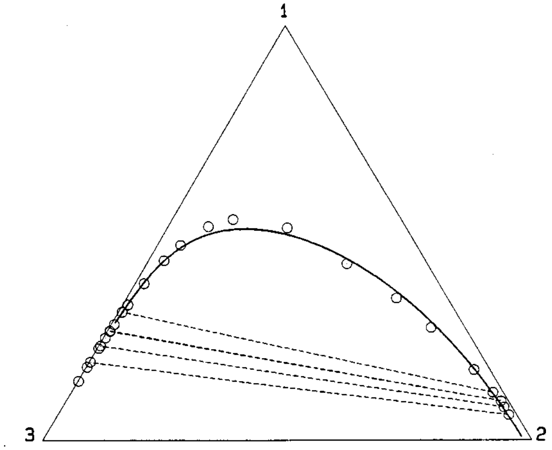

FIG. 17. Phase diagram of the system ethanol (1)—*o*-xylene (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental results of Ref. 2, dashed lines—experimental tie lines, Ref. 2.

References:

[1] W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).

[2] S. Nam, T. Hayakawa, and S. Fujita, J. Chem. Eng. Jpn. **5**, 327 (1972).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *o*-Xylene (1,2-dimethylbenzene, 1,2-xylene); C_8H_{10}; [95-47-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910)

Variables:

T/K=273

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K	x_1	x_2	w_1	w_2
0.0	273.2	0.4153	0.4972	0.2604	0.7182
		0.5053	0.3972	0.3464	0.6275
		0.6030	0.2120	0.5181	0.4198
		0.5977	0.1544	0.5690	0.3388
		0.5873	0.1124	0.6094	0.2687
		0.5580	0.0677	0.6485	0.1814
		0.5252	0.0434	0.6616	0.1259
		0.4615	0.0230	0.6445	0.0739
		0.4116	0.0109	0.6212	0.0379
		0.3232	0.0037	0.5434	0.0142

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogenous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated Error:

accuracy of weighting 0.001 g.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *o*-Xylene (1,2-dimethylbenzene, 1,2-xylene); C_8H_{10}; [95-47-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

S. Nam, T. Hayakawa, and S. Fujita, J. Chem. Eng. Jpn. **5**, 327–34 (1972).

Variables:

T/K = 298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.00	298.15	0.1710	0.7960	0.0847	0.9089
		0.2727	0.6577	0.1502	0.8348
		0.3432	0.5521	0.2072	0.7681
		0.4256	0.4106	0.2964	0.6590
		0.5110	0.2465	0.4353	0.4839
		0.5312	0.1251	0.5568	0.3023
		0.5143	0.0827	0.5963	0.2210
		0.4700	0.0472	0.6124	0.1416
		0.4333	0.0314	0.6060	0.1013
		0.3785	0.0177	0.5774	0.0624
		0.3276	0.0098	0.5377	0.0369
		0.2801	0.0053	0.4900	0.0212
		0.2479	0.0033	0.4521	0.0140
		0.2226	0.0023	0.4192	0.0099
		0.1777	0.0012	0.3543	0.0056
		0.1439	0.0006	0.2999	0.0030

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.061	0.922	0.190	0.002	0.028	0.969	0.372	0.008
		0.080	0.903	0.229	0.003	0.037	0.960	0.428	0.012
		0.095	0.889	0.265	0.004	0.044	0.953	0.472	0.018
		0.095	0.889	0.264	0.005	0.044	0.953	0.471	0.019
		0.116	0.862	0.310	0.007	0.055	0.941	0.522	0.029
		0.102	0.876	0.306	0.008	0.048	0.948	0.517	0.030
		0.130	0.849	0.362	0.014	0.062	0.934	0.566	0.052
		0.147	0.816	0.403	0.023	0.072	0.921	0.592	0.079
		0.167	0.796	0.448	0.036	0.083	0.910	0.611	0.114

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine solubility curve. A binary ethanol–xylene mixture of known composition was prepared in a conical flask with silicone stopper to prevent evaporation. The mixture was placed in a thermostated vessel, agitated by a magnetic stirrer and titrated through a needle of the syringe with water until two phases were observed. The result was checked by another ternary mixture, of the same composition as above: (a) titrated with one of the pure components until the turbidity disappeared, (b) by reappearance of turbidity by lowering the temperature about 0.5 °C. The two-phase mixture was placed in a 50 mL glass-stoppered test tube at temperature of 25 °C, shaken vigorously, kept for nearly 2 h in a constant temperature water bath, and after separation each layer was pipetted for sampling. Refractive index and density of each phase were measured and composition was found from the calibration curves constructed during solubility measurements. When mixtures were not separated clearly after several hours, a centrifuge was used to obtain separation.

Source and Purity of Materials:

(1) Wako Pure Chemical Inst. Ltd., guaranteed reagent; $\rho(25\ °C) = 785.32$ kg m^{-3}, $n(25\ °C,D) = 1.3600$; used as received.
(2) Kishida Chem. Ltd., guaranteed reagent; $\rho(25\ °C) = 870.29$ kg m^{-3}, $n(25\ °C,D) = 1.50175$; used as received.
(3) ion exchanged, distilled.

Estimated Error:

temp. ±0.02 °C and ±0.1 °C (near plait point).

Components:	**Evaluated by:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.04)

4.12. Ethanol + Water + *p*-Xylene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system the system ethanol–*p*-xylene–water is given in Table 35.

TABLE 35. Summary of experimental data for the system ethanol–*p*-xylene–water

Author(s)	T/K	Type of data[a]	Ref.
Bonner, 1909	288	sat. (12)	1
Nam *et al.*, 1972	298	sat. (16), eq. (9)	2
Letcher *et al.*, 1989	298	sat.(15), eq. (6)	3

[a] Number of experimental points in parentheses.

Saturation curve

The system ethanol–*p*-xylene–water forms a miscibility gap of type 1. Solubility data for the saturation curve obtained by the titration method were reported in all three references. Data for phases in equilibrium, reported in Refs. 2 and 3, were also used for construction of the binodal curve. Only one binary pair of components, *p*-xylene–water, is partially miscible. Data of this system were compiled and critically evaluated in a previously published SDS volume.[4] The recommended, values of mutual solubility of *p*-xylene–water system at 298.2 K are: $x_2''=3.1\cdot10^{-5}$ and $x_2'=0.9974$. The end points of the saturation curve, Ref. 3, were reported to be $x_1=0.000$, $x_2=0.998$ and $x_1=0.065$, $x_2=0.000$, which suggests that ethanol is only partially soluble in water. These numerical results are within the accuracy of experimental measurements which was stated by the authors to be 0.005 mole fraction, however, they are not adequate to describe the region of low ethanol concentration. Data of Bonner, Ref. 1, reported at 288.2 K, are consistent with the results of Refs. 2 and 3. All experimental saturation data reported at 298.2 K[2,3] are in agreement. For $x_2>0.003$, the results were fitted to the equation:

$$x_1=0.845\,30+0.111\,30\,\ln(x_2)-0.704\,79x_2-0.144\,88x_2^2.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0246. Selected points on the saturation curve, calculated by this equation together with the ''best'' values of Ref. 4 are presented in Table 36. Experimental points at 298.2 K are also presented in Fig. 18.

TABLE 36. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 031 Ref. 4	0.3795	0.5000
0.0758	0.0010	0.3668	0.5200
0.3257	0.0100	0.3539	0.5400
0.3957	0.0200	0.3406	0.5600
0.4586	0.0400	0.3272	0.5800
0.4894	0.0600	0.3134	0.6000
0.5069	0.0800	0.2994	0.6200
0.5171	0.1000	0.2852	0.6400
0.5226	0.1200	0.2708	0.6600
0.5250	0.1400	0.2561	0.6800
0.5249	0.1600	0.2413	0.7000
0.5229	0.1800	0.2262	0.7200
0.5194	0.2000	0.2109	0.7400
0.5147	0.2200	0.1954	0.7600
0.5090	0.2400	0.1798	0.7800
0.5023	0.2600	0.1639	0.8000
0.4949	0.2800	0.1479	0.8200
0.4868	0.3000	0.1316	0.8400
0.4781	0.3200	0.1152	0.8600
0.4688	0.3400	0.0987	0.8800
0.4591	0.3600	0.0819	0.9000
0.4489	0.3800	0.0650	0.9200
0.4382	0.4000	0.0479	0.9400
0.4272	0.4200	0.0306	0.9600
0.4158	0.4400	0.0132	0.9800
0.4040	0.4600	0.0044	0.9900
0.3919	0.4800	0.0000	0.9974 Ref. 4

Phases in equilibrium

Compositions of equilibrium phases of the ternary system ethanol–*p*-xylene–water at 298.2 K were reported in Refs. 2 and 3. These data are presented in Fig. 18. The reported tie lines cross one another. For similar compositions of the hydrocarbon-rich phase, the concentration of ethanol at equilibrium in the water-rich phase is always reported to be lower by Nam *et al.*,[2] than by Letcher *et al.*,[3] e.g.: $x_1'=0.044$ $x_2'=0.939$, $x_1''=0.0728$ $x_2''=0.0004$ (Ref. 2) and $x_1'=0.031$ $x_2'=0.960$, $x_1''=0.0292$ $x_2''=0.0007$ (Ref. 3) or $x_1'=0.163$ $x_2'=0.806$, $x_1''=0.4457$ $x_2''=0.0369$ (Ref. 2) and $x_1'=0.168$ $x_2'=0.795$, $x_1''=0.514$ $x_2''=0.074$ (Ref. 3). These equilibrium data sets are not consistent with one another, although each is internally consistent. The plait point of the system at 298.2 K, calculated by Letcher and Siswana[5] was reported to be $x_1=0.48$ $x_2=0.35$. The plait point reported by Bonner at 288.2 K[1] was $x_1=0.486$, $x_2=0.340$. The equilibrium and saturation data are presented together with calculated binodal curve in Fig. 18.

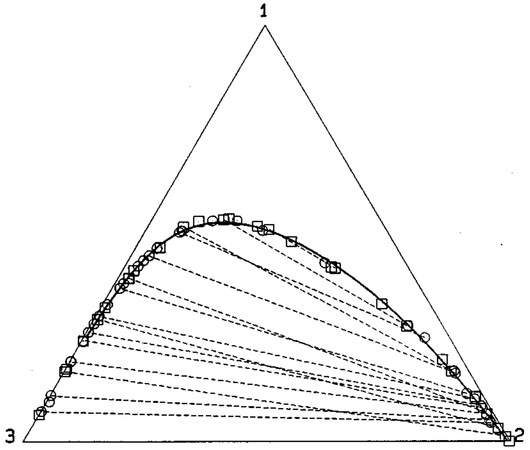

FIG. 18. Phase diagram of the system ethanol (1)—*p*-xylene (2)—water (3) at 298.2 K. Solid line—calculated binodal curve, ○—experimental results of Ref. 2, □—experimental results of Ref. 3, dashed lines—experimental tie lines, Refs. 2 and 3.

References:

[1] W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).

[2] S. Nam, T. Hayakawa, and S. Fujita, J. Chem. Eng. Jpn. **5**, 327 (1972).

[3] T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

[4] D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

[5] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910).

Variables:

T/K=273

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2	
		(compiler)		(compiler)		
15.0	288.2	0.3768	0.5161	0.2343	0.7397	
		0.4732	0.3581	0.3468	0.6048	
		0.4856	0.3401	0.3631	0.5860	plait point
		0.5238	0.2629	0.4318	0.4994	
		0.5532	0.1734	0.5220	0.3772	
		0.5572	0.1318	0.5671	0.3091	
		0.5280	0.0630	0.6337	0.1744	
		0.5040	0.0464	0.6407	0.1358	
		0.4753	0.0353	0.6354	0.1086	
		0.4308	0.0222	0.6190	0.0735	
		0.3625	0.0103	0.5741	0.0375	

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogenous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated Error:

accuracy of weighing 0.0001 g.

Components:
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
S. Nam, T. Hayakawa, and S. Fujita, J. Chem. Eng. Jpn. **5**, 327–34 (1972).

Variables:
$T/K=298$

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.00	298.15	0.1685	0.8004	0.0832	0.9108
		0.2750	0.6529	0.1521	0.8323
		0.0963	0.0050	0.2097	0.0250
		0.4276	0.4062	0.2993	0.6552
		0.5057	0.2401	0.4365	0.4777
		0.5297	0.1761	0.5042	0.3863
		0.5292	0.1257	0.5548	0.3037
		0.5049	0.0755	0.5990	0.2063
		0.4636	0.0441	0.6119	0.1340
		0.4206	0.0266	0.6025	0.0879
		0.4339	0.0309	0.6073	0.0998
		0.3789	0.0175	0.5783	0.0615
		0.3277	0.0096	0.5381	0.0364
		0.2815	0.0052	0.4918	0.0208
		0.2399	0.0028	0.4423	0.0117
		0.1930	0.0015	0.3774	0.0066

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/°C$	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.044	0.939	0.0728	0.0004	0.020	0.977	0.167	0.002
		0.051	0.932	0.1113	0.0006	0.023	0.974	0.242	0.003
		0.066	0.918	0.1917	0.0011	0.030	0.967	0.376	0.005
		0.080	0.903	0.2413	0.0028	0.037	0.960	0.444	0.012
		0.086	0.897	0.2613	0.0036	0.040	0.957	0.469	0.015
		0.102	0.876	0.3000	0.0064	0.048	0.948	0.512	0.025
		0.115	0.853	0.3671	0.0154	0.055	0.939	0.570	0.055
		0.163	0.806	0.4457	0.0369	0.080	0.914	0.608	0.116
		0.247	0.701	0.5013	0.0720	0.131	0.858	0.601	0.199

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine solubility curve. A binary ethanol–xylene mixture of known composition was prepared in a conical flask with silicone stopper to prevent evaporation. The mixture was placed in a thermostated vessel, agitated by a magnetic stirrer and titrated through a needle of the syringe with water until two phases were observed. The result was checked by another ternary mixture, of the same composition as above: (a) titrated with one of the pure components until the turbidity disappeared, (b) by reappearance of turbidity by lowering the temperature about 0.5 °C. The two-phase mixture was placed in a 50 mL glass-stoppered test tube at temperature of 25 °C, shaken vigorously, kept for nearly 2 h in a constant temperature water bath, and after separation each layer was pipetted for sampling. Refractive index and density of each phase were measured and composition was found from the calibration curves constructed during solubility measurements. When mixtures were not separated clearly after several hours, a centrifuge was used to obtain separation.

Source and Purity of Materials:

(1) Wako Pure Chemical Inst. Ltd., guaranteed reagent; $\rho(25\ °C)=785.32\ kg\ m^{-3}$, $n(25\ °C,D)=1.3600$; used as received.
(2) Kishida Chem. Ltd., guaranteed reagent; $\rho(25\ °C)=856.65\ kg\ m^{-3}$, $n(25\ °C,D)=1.4916$; used as received.
(3) ion exchanged, distilled.

Estimated Error:

temp. ±0.02 °C and ±0.1 °C (near plait point).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053–60 (1989).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.998	0.000	0.9997
		0.107	0.875	0.050	0.946
		0.196	0.763	0.099	0.892
		0.328	0.572	0.195	0.782
		0.418	0.424	0.287	0.671
		0.479	0.312	0.374	0.562
		0.516	0.224	0.455	0.455
		0.534	0.157	0.525	0.356
		0.528	0.098	0.587	0.251
		0.465	0.050	0.604	0.150
		0.410	0.023	0.599	0.077
		0.320	0.008	0.532	0.031
		0.241	0.003	0.443	0.013
		0.174	0.001	0.349	0.005
		0.065	0.000	0.151	0.000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C (compiler)	T/K	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.415	0.433	0.508	0.252	0.282	0.678	0.430	0.491
		0.275	0.650	0.532	0.147	0.153	0.831	0.534	0.340
		0.168	0.795	0.514	0.074	0.083	0.909	0.608	0.202
		0.066	0.919	0.391	0.022	0.030	0.967	0.582	0.076
		0.031	0.960	0.292	0.007	0.014	0.985	0.501	0.028
		0.011	0.985	0.168	0.001	0.005	0.994	0.339	0.005

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. A binary mixture of known composition was titrated with the third component until cloudiness was observed. Tie line compositions were related to the coexistence curve; water was determined by the Karl Fischer titration. The methods were described in Ref. 1.

Source and Purity of Materials:

(1) source not specified; used as received.
(2) source not specified; recrystallized three times.
(3) not specified.

Estimated Error:

comp. <0.005 mole fraction (estimated authors' precision on binodal curve), <0.01 mole fraction (estimated authors' precision of tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) 2,4,4-Trimethyl-1-pentene (alpha-diisobutylene); C_8H_{16}; [107-39-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130–2 (1945).

Variables:

T/K=228–298

Compiled by:

A. Skrzecz

4.13. Ethanol + Water + 2,4,4-Trimethyl-1-pentene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
−45.0	228.2	0.6682	0.2471	0.5127	0.4619
		0.4515	0.5010	0.2671	0.7219
0.0	273.2	0.6242	0.2309	0.5021	0.4523
		0.4355	0.4832	0.2648	0.7158
25.0	298.2	0.5984	0.2213	0.4954	0.4463
		0.4258	0.4725	0.2634	0.7120

Comments and Additional Data

Water tolerance (S) was described with probable error $<0.5\%$ at the range −45–25 °C by the equation: $\log(S)=a-b/(T/\mathrm{K})$. The parameters ($a$, b) were determined from plots. Water tolerance was defined as: $S=H_2O$ % by volume·(100−Hydrocarbon % by volume in the blend)/100.

vol % hydrocarbon	a	b
75	1.400	340.3
50	1.842	355.4

Auxiliary Information

Method/Apparatus/Procedure:

A glass tube with stirrer containing the ternary mixture was immersed in a bath, the temperature of which could be varied. Mixtures were prepared directly in the tube, by special pipettes at 15.5 °C. Precautions to exclude moisture and to prevent evaporation were observed. No correction was made for the slight expansion in volume when alcohol was mixed with hydrocarbon. In the paper the experimental results were expressed as the water tolerance of the alcohol–hydrocarbon blend. For practical purposes water tolerance was defined as the volume percent of water which can be added before separation occurs.

Source and Purity of Materials:

(1) source not specified; anhydrous ethanol.
(2) source not specified.
(3) not specified.

Estimated Error:

temp. within about 0.3 °C (duplicate determinations), composition <0.2% relative of volume fraction.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) 1-Octene; C_8H_{16}; [111-66-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

J. Nowakowska, C. B. Kretschmer, and R. Wiebe, J. Chem. Eng. Data Ser. **1**, 42–5 (1956).

Variables:

T/K=273–298

Compiled by:

A. Skrzecz

4.14. Ethanol + Water + 1-Octene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
0.0	273.2	0.0329	0.0000	0.080	0.000
		0.0515	0.0000	0.122	0.000
		0.0712	0.0000	0.164	0.000
		0.1164	0.0000	0.252	0.000
		0.1702	0.0000	0.344	0.000
		0.1967	0.0000	0.385	0.000
		0.2288	0.0002	0.431	0.001
		0.2472	0.0002	0.456	0.001
		0.2900	0.0005	0.510	0.002
		0.3610	0.0015	0.588	0.006
		0.4352	0.0041	0.655	0.015
		0.4720	0.0057	0.684	0.020
		0.6121	0.0230	0.755	0.069
		0.6821	0.0504	0.750	0.135
		0.6972	0.0650	0.735	0.167
		0.7073	0.1311	0.649	0.293
		0.6514	0.2406	0.509	0.458
		0.5339	0.3958	0.350	0.632
		0.3476	0.6144	0.187	0.805
20.0	298.2	0.0329	0.0000	0.080	0.000
		0.0515	0.0000	0.122	0.000
		0.0712	0.0000	0.164	0.000
		0.1164	0.0000	0.252	0.000
		0.1477	0.0000	0.307	0.000
		0.1508	0.0002	0.312	0.001
		0.1989	0.0002	0.388	0.001
		0.2240	0.0004	0.424	0.002
		0.2841	0.0009	0.502	0.004
		0.3837	0.0036	0.607	0.014
		0.4195	0.0054	0.638	0.020
		0.4701	0.0089	0.676	0.031
		0.5395	0.0161	0.717	0.052
		0.5606	0.0210	0.723	0.066
		0.6038	0.0340	0.729	0.100
		0.6560	0.0609	0.717	0.162
		0.6726	0.1248	0.637	0.288
		0.6202	0.2307	0.500	0.453
		0.5205	0.3874	0.347	0.629
		0.3332	0.6148	0.180	0.809

Compositions of coexisting phases

$t/°C$	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
0.0	273.2	0.005	0.995	0.1396	0.0002	0.002	0.998	0.293	0.001
		0.012	0.988	0.2334	0.0004	0.005	0.995	0.437	0.002
		0.019	0.981	0.3717	0.0015	0.008	0.992	0.599	0.006
		0.043	0.957	0.4807	0.0063	0.018	0.982	0.690	0.022
		0.068	0.927	0.5884	0.0188	0.029	0.970	0.747	0.058
		0.131	0.857	0.6996	0.0697	0.059	0.939	0.729	0.177
20.0	298.2	0.000	1.000	0.0566	0.0000	0.000	1.000	0.133	0.000
		0.010	0.984	0.1309	0.0000	0.004	0.995	0.278	0.000
		0.017	0.977	0.2358	0.0000	0.007	0.992	0.441	0.000
		0.033	0.955	0.3020	0.0012	0.014	0.984	0.523	0.005
		0.062	0.920	0.4687	0.0083	0.027	0.970	0.676	0.029
		0.105	0.872	0.5861	0.0263	0.047	0.949	0.731	0.080
		0.139	0.833	0.6303	0.0456	0.064	0.931	0.726	0.128
		0.222	0.731	0.6734	0.0932	0.110	0.881	0.679	0.229

Auxiliary Information

Method/Apparatus/Procedure:

Points on the binodal curve were obtained by titrating a known mixture of two components by the third component until turbidity appeared or disappeared. The mixtures were prepared by volume with calibrated pipettes and the results converted to weight percent. Over most of the composition range alcohol–hydrocarbon mixtures were titrated with water. For 25 °C, the end point was taken when the the mixture remained homogenous at 25.0 °C, but become turbid at 24.8 °C. The titrations at 0 °C were performed in small conical flasks with magnetic stirrers placed in Dewar vessel. Tie lines were determined through measurements of refractive index at 25 °C of both phases in equilibrium and comparison with the values obtained on binodal curve. For saturated solutions containing more than 40% ethanol the tie lines were obtained by measuring densities at 25 °C in a similar procedure. The experimental procedures were adapted mainly from Ref. 1.

Source and Purity of Materials:

(1) source not specified, commercial absolute grade; used as received; $\rho(25\ °C)=785.97$ kg m^{-3}, water concentration 0.30 mass % (water was taken into account in calculations of composition).
(2) Philips, pure grade purity >99 mole %; used as received; $\rho(25\ °C)=710.78$ kg m^{-3}.
(3) distilled.

Estimated Error:

conc. $<0.1\%$ (relative error) for ethanol in the region near 100% of hydrocarbon (tie lines).

References:

[1] E. R. Washburn, V. Hnizda, and R. Vold, J. Am. Chem. Soc. **53**, 3237 (1931)

Components:	**Evaluated by:**
(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5] (2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1] (3) Water (hydrogen oxide); H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.05)

4.15. Ethanol + Water + 2,2,4-Trimethylpentane

Critical Evaluation:

A survey of reported in the literature compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system ethanol–2,2,4-trimethylpentane–water is given in Table 37.

TABLE 37. Summary of experimental data for the system ethanol–2,2,4-trimethylpentane–water

Author(s)	T/K	Type of data[a]	Ref.
Kretschmer and Wiebe, 1945	228–298	sat. (12)	1
Nowakowska *et al.*, 1956	273–298	sat. (50), eq. (14)	2
Huber *et al.*, 1972	298	eq. (6)	3

[a] Number of experimental points in parentheses.

Saturation curve

The system ethanol–2,2,4-trimethylpentane–water forms a miscibility gap of type 1. Experimental points on the saturation curve were reported by Kretschmer and Wiebe[1] and Nowakowska *et al.*[2] In both references the saturation curves were obtained by the titration method. In Ref. 1 the experimental results at 228, 273, and 298 K were expressed as the water tolerance of the alcohol–hydrocarbon mixture. The binary 2,2,4-trimethylpentane–water system is only partially miscible. The data for this system were compiled and critically evaluated in a previously published SDS volume,[4] the binary solubility data were not reported together with ternary data in any of the references. The ''best'' (Ref. 4) values of mutual solubility at 293 and 298 K are: $x''_2=3\cdot 10^{-7}$, $x'_2=0.9995$ and $x''_2=3.5\cdot 10^{-7}$, $x'_2=0.9994$, respectively. Compositions of coexisting phases in equilibrium at 273 and 298 K (Refs. 2 and 3) were included and also used for data comparison on saturation curves. All data sets are consistent with one another. The temperature relationship of miscibility gap, (Refs. 1 and 2) is as expected one. At higher temperatures smaller miscibility gaps are found. The water-rich phase with low concentrations of ethanol ($x_1<0.20$), Ref. 2, was reported to be 2,2,4-trimethylpentane free, presumably due to the analytical methods used. The maximum ethanol concentration is observed on the saturation curve. At 298.2 K it reaches $x_1=0.71\pm 0.01$ when $x_2=0.10\pm 0.02$ mole fraction. All experimental solubility and equilibrium data reported at 298.2 K were used for calculation of the saturation curve. (Water-rich and hydrocarbon-rich branches were treated together.) These data were described by the equation:

$$x_1=1.021\,78+0.104\,50\ \ln(x_2)-1.018\,38x_2\,.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0243. This equation describes the saturation curve for $x_2<0.95$ mole fraction. The points on the saturation curve, calculated by the above equation together with the ''best'' values from Ref. 4 are presented in Table 38 for selected concentration of 2,2,4-trimethylpentane in the mixture and in Fig. 19 as calculated binodal curve (solid line).

TABLE 38. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	$3.5\cdot 10^{-7}$ Ref. 4	0.4563	0.4800
0.2989	0.0010	0.4402	0.5000
0.5303	0.0100	0.4239	0.5200
0.5926	0.0200	0.4075	0.5400
0.6447	0.0400	0.3909	0.5600
0.6667	0.0600	0.3742	0.5800
0.6764	0.0800	0.3574	0.6000
0.6793	0.1000	0.3404	0.6200
0.6780	0.1200	0.3234	0.6400
0.6737	0.1400	0.3062	0.6600
0.6673	0.1600	0.2890	0.6800
0.6593	0.1800	0.2716	0.7000
0.6499	0.2000	0.2542	0.7200

0.6395	0.2200	0.2367	0.7400
0.6282	0.2400	0.2191	0.7600
0.6162	0.2600	0.2015	0.7800
0.6036	0.2800	0.1838	0.8000
0.5904	0.3000	0.1660	0.8200
0.5768	0.3200	0.1481	0.8400
0.5628	0.3400	0.1302	0.8600
0.5484	0.3600	0.1122	0.8800
0.5337	0.3800	0.0942	0.9000
0.5187	0.4000	0.0762	0.9200
0.5034	0.4200	0.0580	0.9400
0.4879	0.4400	0.0535	0.9500
0.4722	0.4600	0.0000	0.9994 Ref. 4

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system ethanol–2,2,4-trimethylpentane–water were presented in Refs. 2 and 3 and the reported tie lines cover the whole range of the miscibility gap. They were obtained by various analytical methods: refractive indexes, Ref. 2, or by glc, Ref. 3. The direction of tie lines differ slightly. They may be treated as tentative. Experimental tie lines together with all experimental saturation points at 298.2 K are presented in Fig. 19.

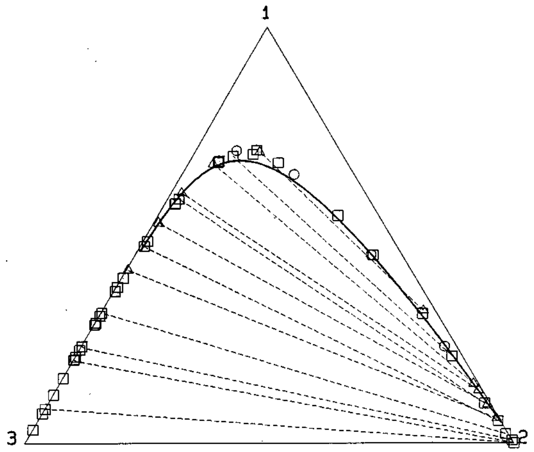

FIG. 19. Phase diagram of the system ethanol (1)—2,2,4-trimethylpentane (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 1, □—experimental data, Ref. 2, △—experimental data, Ref. 3, dashed lines—experimental tie lines, Refs. 2 and 3.

References:

[1] C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130 (1945).
[2] J. Nowakowska, C. B. Kretschmer, and R. Wiebe, J. Chem. Eng. Data Ser. **1**, 42 (1956).
[3] J. F. K. Huber, C. A. M. Meijers, J. A. R. J. Hulsman, Anal. Chem. **44**, 111 (1972).
[4] D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) 2, 2, 4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

C. B. Kretschmer and R. Wiebe, Ind. Eng. Chem. **37**, 1130–2 (1945).

Variables:

T/K=228–298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

		x_1	x_2	w_1	w_2
t/°C	T/K (compiler)	(compiler)		(compiler)	
−45.0	228.2	0.8028	0.0957	0.7434	0.2198
		0.7070	0.2529	0.5238	0.4646
		0.4737	0.5085	0.2720	0.7240
		0.2353	0.7578	0.1112	0.8876
0.0	273.2	0.7397	0.0882	0.7212	0.2132
		0.6709	0.2400	0.5157	0.4575
		0.4612	0.4950	0.2704	0.7196
		0.2329	0.7500	0.1110	0.8859
25.0	298.2	0.7032	0.0839	0.7072	0.2091
		0.6454	0.2309	0.5097	0.4521
		0.4517	0.4848	0.2691	0.7161
		0.2310	0.7438	0.1108	0.8845

Comments and Additional Data

Water tolerance (S) was described with probable error <0.5% at the range −45–25 °C by the equation: $\log(S)=a-b/(T/\mathrm{K})$. The parameters ($a,b$) were determined from plots. Water tolerance was defined as: $S=H_2O$ % by volume·(100-Hydrocarbon % by volume in the blend)/100

vol % hydrocarbon	a	b
90	1.383	553.5
75	1.894	554.5
50	2.151	504.4
25	2.001	352.5

Auxiliary Information

Method/Apparatus/Procedure:

A glass tube with stirrer containing the ternary mixture was immersed in a bath, the temperature of which could be varied. Mixtures were prepared directly in the tube, by special pipettes at 15.5 °C. Precautions to exclude moisture and to prevent evaporation were observed. No correction was made for the slight expansion in volume when alcohol was mixed with hydrocarbon. In the paper the experimental results were expressed as the water tolerance of the alcohol–hydrocarbon blend. For practical purposes water tolerance was defined as the volume per cent of water which can be added before separation occurs.

Source and Purity of Materials:

(1) source not specified; anhydrous ethanol.
(2) source not specified; b.p.=99.25 °C.
(3) not specified.

Estimated Error:

temp. within about 0.3 °C (duplicate determinations), composition <0.2% relative of volume fraction.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

J. Nowakowska, C. B. Kretschmer, and R. Wiebe, J. Chem. Eng. Data Ser. **1**, 42–5 (1956).

Variables:

T/K=273–298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
0.0	273.2	0.0515	0.0000	0.122	0.000
		0.1164	0.0000	0.252	0.000
		0.1733	0.0000	0.349	0.000
		0.1894	0.0000	0.374	0.000
		0.2216	0.0002	0.421	0.001
		0.2472	0.0002	0.456	0.001
		0.2746	0.0005	0.491	0.002
		0.2770	0.0005	0.494	0.002
		0.3539	0.0012	0.581	0.005
		0.3654	0.0012	0.593	0.005
		0.4196	0.0029	0.643	0.011
		0.4218	0.0029	0.645	0.011
		0.5320	0.0095	0.724	0.032
		0.5361	0.0095	0.727	0.032
		0.5697	0.0133	0.744	0.043
		0.5764	0.0137	0.748	0.044
		0.6289	0.0225	0.766	0.068
		0.6421	0.0227	0.774	0.068
		0.6587	0.0293	0.772	0.085
		0.7213	0.0642	0.748	0.165
		0.7335	0.1302	0.661	0.291
		0.7104	0.1871	0.585	0.382
		0.6727	0.2348	0.521	0.451
		0.6126	0.3147	0.431	0.549
		0.5030	0.4430	0.310	0.677
		0.3543	0.6166	0.187	0.807
20.0	298.2	0.0329	0.0000	0.080	0.000
		0.0712	0.0000	0.164	0.000
		0.1164	0.0000	0.252	0.000
		0.1556	0.0002	0.320	0.001
		0.2002	0.0002	0.390	0.001
		0.2066	0.0004	0.399	0.002
		0.2226	0.0004	0.422	0.002
		0.2833	0.0009	0.501	0.004
		0.2882	0.0009	0.507	0.004
		0.3045	0.0012	0.526	0.005
		0.3639	0.0025	0.589	0.010
		0.3742	0.0023	0.600	0.009
		0.3960	0.0036	0.619	0.014
		0.4848	0.0088	0.688	0.031
		0.5746	0.0205	0.733	0.065
		0.5760	0.0206	0.734	0.065
		0.6747	0.0598	0.728	0.160
		0.6780	0.0604	0.729	0.161
		0.7042	0.1246	0.652	0.286
		0.6942	0.1225	0.649	0.284
		0.6734	0.1841	0.568	0.385
		0.5460	0.3698	0.365	0.613
		0.4504	0.4892	0.267	0.719
		0.3095	0.6604	0.158	0.836

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
0.0	273.2	0.007	0.993	0.2331	0.0002	0.003	0.997	0.437	0.001
		0.022	0.978	0.3771	0.0018	0.009	0.991	0.604	0.007
		0.029	0.972	0.4737	0.0053	0.012	0.988	0.686	0.019
		0.057	0.937	0.5922	0.0152	0.024	0.975	0.756	0.048
		0.113	0.881	0.7044	0.0529	0.049	0.950	0.757	0.141
		0.150	0.839	0.7352	0.0760	0.067	0.931	0.737	0.189
		0.222	0.762	0.7274	0.1544	0.105	0.892	0.629	0.331
20.0	298.2	0.000	1.000	0.0825	0.0000	0.000	1.000	0.187	0.000
		0.000	1.000	0.1989	0.0002	0.000	1.000	0.388	0.001
		0.007	0.993	0.2310	0.0009	0.003	0.997	0.433	0.004
		0.022	0.972	0.3114	0.0012	0.009	0.990	0.534	0.005
		0.053	0.941	0.4729	0.0079	0.022	0.977	0.680	0.028
		0.095	0.893	0.5865	0.0228	0.041	0.957	0.737	0.071
		0.208	0.770	0.6903	0.0830	0.098	0.898	0.701	0.209

Auxiliary Information

Method/Apparatus/Procedure:

Points on the binodal curve were obtained by titrating a known mixture of two components by the third component until turbidity appeared or disappeared. The mixtures were prepared by volume with calibrated pipettes and the results converted to weight percent. Over most of the composition range alcohol–hydrocarbon mixtures were titrated with water. For 25 °C, the end point was taken when the the mixture remained homogenous at 25.0 °C, but become turbid at 24.8 °C. The titrations at 0 °C were performed in small conical flasks with magnetic stirrers placed in Dewar vessel. The lines were determined through measurements of refractive index at 25 °C of both phases in equilibrium and comparison with the values obtained on binodal curve. For saturated solutions containing more than 40% ethanol the tie lines were obtained by measuring densities at 25 °C in a similar procedure. The experimental procedures were adapted mainly from Ref. 1.

Source and Purity of Materials:

(1) source not specified, commercial absolute grade; used as received; $\rho(25\ ^\circ\mathrm{C})=785.97\ \mathrm{kgm}^{-3}$, water concentration 0.30 mass % (water was taken into account in calculations of composition).
(2) source not specified, certified knock-rating grade; distilled to remove olefins, filtered by silica gel; $\rho(25\ ^\circ\mathrm{C})=687.74\ \mathrm{kg\ m}^{-3}$.
(3) distilled.

Estimated Error:

conc.<0.1% (relative error) for ethanol in the region near 100% of hydrocarbon (tie lines).

References

[1] E. R. Washburn, V. Hnizda, and R. Vold, J. Am. Chem. Soc. **53**, 3237 (1931).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) 2, 2, 4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

J. F. K. Huber, C. A. M. Meijers, and J. A. R. J. Hulsman, Anal. Chem. **44**, 111–6 (1972).

Variables:

$T/\mathrm{K}=298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

$t/°\mathrm{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.317	0.658	0.700	0.133	0.162	0.833	0.639	0.301
		0.142	0.847	0.671	0.051	0.063	0.935	0.740	0.140
		0.126	0.865	0.601	0.021	0.055	0.943	0.750	0.065
		0.093	0.900	0.529	0.009	0.040	0.959	0.723	0.030
		0.059	0.935	0.416	0.003	0.025	0.974	0.639	0.011
		0.037	0.961	0.296	0.002	0.015	0.984	0.514	0.009

Auxiliary Information

Method/Apparatus/Procedure:

Equilibrium was established in a thermostated vessel with a magnetic stirrer and the composition of each of the phases was determined analytically by glc. Data were obtained during measurements of partition coefficients for steroids in liquid–liquid systems.

Source and Purity of Materials:

(1) Merck Uvasole, spectroquality grade; used as received.
(2) Merck Uvasole, spectroquality grade; used as received.
(3) double distilled.

Estimated Error:

temp. ±0.1 °C.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Octane (*n*-octane); C_8H_{18} ; [111-65-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40** 3018-23 (1966). [Eng. transl. Russ. J. Phys. Chem. **40**, 1619–22 (1966)].

Variables:

$T/\mathrm{K}=298$

Compiled by:

A. Skrzecz

4.16. Ethanol + Water + Octane

Experimental Data

Compositions along the saturation curve

$t/°\mathrm{C}$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9937	0.000	0.999
		0.3330	0.6374	0.173	0.821
		0.4845	0.4687	0.291	0.698
		0.6099	0.3172	0.428	0.552
		0.7023	0.2052	0.563	0.408
		0.7121	0.1830	0.590	0.376
		0.7449	0.1319	0.665	0.292
		0.7382	0.1196	0.677	0.272
		0.7339	0.0808	0.729	0.199
		0.7242	0.0670	0.745	0.171
		0.7240	0.0620	0.753	0.160
		0.6986	0.0452	0.767	0.123
		0.6756	0.0353	0.771	0.100
		0.5998	0.0173	0.757	0.054
		0.5169	0.0097	0.712	0.033
		0.4945	0.0068	0.700	0.024
		0.4521	0.0055	0.667	0.020
		0.2697	0.0009	0.484	0.004
		0.2191	0.0004	0.417	0.002
		0.1792	0.0002	0.358	0.001

Compositions of coexisting phases

$t/°\mathrm{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.000	1.000	0.472	0.006	0.000	1.000	0.684	0.020
		0.067	0.933	0.621	0.021	0.028	0.972	0.764	0.064
		0.106	0.888	0.680	0.037	0.046	0.953	0.770	0.105
		0.164	0.825	0.739	0.077	0.074	0.924	0.738	0.190
		0.351	0.624	0.714	0.186	0.184	0.811	0.588	0.380
		0.418	0.546	0.674	0.243	0.234	0.758	0.515	0.460
		0.493	0.461	0.622	0.306	0.298	0.691	0.442	0.538
		0.553	0.388	0.553	0.388	0.360	0.625	0.360	0.625

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, Ref. 1, was used to determine solubility of the mixtures. The third component was added to the binary homogenous mixture until cloudiness was first observed. Density of the saturated mixtures was measured; these results were graphed. To obtain equilibrium, ternary mixtures were stirred in a thermostated vessel for several hours. After phase separation, the density of each phase was measured and composition was determined from the graphs prepared earlier. Concentration at the critical point was found by method described in Ref. 2. Water included in ethanol was taken into account in all measurements.

Source and Purity of Materials:

(1) source not specified, ‘‘rectificate grade;’’ distilled; water concentration was determined by the Karl Fischer method.
(2) source not specified; b.p. = 125.5 °C, $n(20\ °\text{C,D}) = 1.3976$.
(3) not specified.

Estimated Error:

solubility ±0.001 mass fraction.

References

[1] W. D. Bancroft, Phys. Rev. **3**, 21 (1896).
[2] E. N. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12}; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.05)

4.17. Ethanol + Water + Mesitylene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system ethanol–mesitylene–water is given in Table 39.

TABLE 39. Summary of experimental data for the system ethanol–mesitylene–water

Author(s)	T/K	Type of data[a]	Ref.
Bonner, 1909	273	sat. (10)	1
Letcher *et al.*, 1992	298	sat. (15), eq. (7)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system ethanol–mesitylene–water forms a miscibility gap of type 1. Data for the system were reported in two references and are evaluated on the basis of the original papers. Only one binary system mesitylene–water forms a miscibility gap. This system was compiled and critically evaluated in a previously published SDS volume.[3] The recommended value at 298 K is $x_2' = 7.4 \cdot 10^{-6}$; solubility of water in mesitylene was not reported. The miscibility gap reported by Bonner[1] at 273 K is larger than the one at 298 K, which is in agreement with general expectation. Experimental errors estimated by evaluator are ±0.0005 mole fraction for data reported in Ref. 1. The authors of Ref. 2 estimated their errors at 0.005 mole fraction for the binodal curve and 0.01 mole fraction for tie line compositions. Mutual solubility data for the misytylene–water system reported at 298.2 K together with the ternary data,[2] are $x_2' = 0.000$ and $x_2'' = 0.999$. They differ significantly from recommended values but are within the accuracy of experimental measurements. Data are consistent within each data set as well as between sets and are considered tentative. Data reported at 298.2 K by Letcher *et al.*[2] were described by the equation:

$$x_1 = 0.935\,36 + 0.113\,49\ \ln(x_2) - 0.889\,03 x_2 - 0.049\,05 x_2^2.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0082. Selected points on the saturation curve, calculated by the above equation together with the recommended value of Ref. 3 are presented in Table 40.

TABLE 40. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	$7.4 \cdot 10^{-6}$ Ref. 3	0.3999	0.5000
0.1505	0.0010	0.3856	0.5200
0.4038	0.0100	0.3710	0.5400
0.4736	0.0200	0.3563	0.5600
0.5344	0.0400	0.3414	0.5800
0.5625	0.0600	0.3263	0.6000
0.5773	0.0800	0.3111	0.6200
0.5846	0.1000	0.2956	0.6400
0.5873	0.1200	0.2801	0.6600
0.5868	0.1400	0.2644	0.6800
0.5839	0.1600	0.2485	0.7000
0.5791	0.1800	0.2325	0.7200
0.5729	0.2000	0.2164	0.7400
0.5656	0.2200	0.2002	0.7600
0.5572	0.2400	0.1839	0.7800
0.5480	0.2600	0.1674	0.8000
0.5381	0.2800	0.1509	0.8200
0.5276	0.3000	0.1342	0.8400

0.5165	0.3200	0.1174	0.8600
0.5050	0.3400	0.1005	0.8800
0.4930	0.3600	0.0835	0.9000
0.4806	0.3800	0.0665	0.9200
0.4679	0.4000	0.0493	0.9400
0.4549	0.4200	0.0321	0.9600
0.4415	0.4400	0.0147	0.9800
0.4279	0.4600	0.0060	0.9900
0.4140	0.4800	0.0000	0.9990 Ref. 2

Phases in equilibrium

Equilibrium data for the ternary system ethanol–mesitylene–water were reported at 298.2 K only by Letcher *et al.*[2] They are consistent within the series. The plait point calculated by the authors (Ref. 2) was $x_1=0.50$, $x_2=0.35$, while the maximum concentration of ethanol on binodal curve was $x_1=0.60$. The plait point reported by Bonner at 273.2 K.[1] was $x_1=0.517$, $x_2=0.400$. The experimental data for phase equilibria are treated as tentative and are presented together with experimental points on saturation curve in Fig. 20.

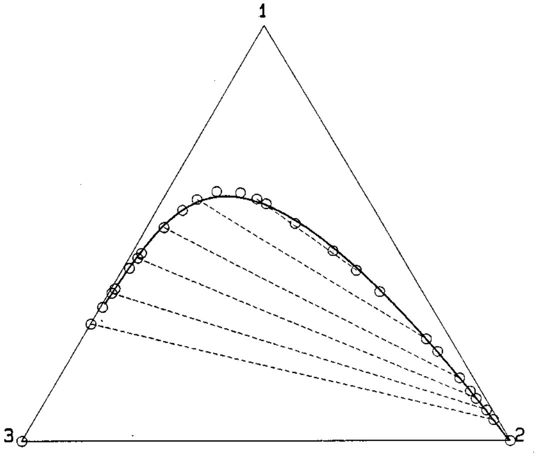

FIG. 20. Phase diagram of the system ethanol-mesitylene-water at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 2.

References:

[1]W. D. Bonner, J. Phys. Chem. **14**, 738 (1909–1910).

[2]T. M. Letcher and P. M. Siswana, Fluid Phase Equilib, **74**, 203 (1992).

[3]D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12} ; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910)

Variables:

T/K=273

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2	w_1 (compiler)	w_2	
0.0	273.2	0.5170	0.4004	0.3243	0.6554	plait point
		0.5267	0.3767	0.3404	0.6352	
		0.6289	0.2236	0.4952	0.4594	
		0.6657	0.1448	0.5956	0.3381	
		0.6632	0.0879	0.6700	0.2317	
		0.6425	0.0595	0.7028	0.1697	
		0.5797	0.0238	0.7275	0.0779	
		0.5396	0.0165	0.7135	0.0570	
		0.5007	0.0091	0.6992	0.0331	
		0.3977	0.0048	0.6176	0.0195	

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogeneous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated Error:

accuracy of weighing 0.0001 g.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12}; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Original measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17. (1992).

Variables:

T/K = 298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.322	0.004	0.540	0.018
		0.367	0.007	0.582	0.029
		0.416	0.012	0.620	0.047
		0.452	0.019	0.638	0.070
		0.554	0.053	0.655	0.163
		0.599	0.101	0.611	0.269
		0.596	0.152	0.546	0.363
		0.569	0.218	0.466	0.466
		0.522	0.300	0.380	0.570
		0.457	0.409	0.290	0.677
		0.359	0.553	0.196	0.786
		0.215	0.743	0.099	0.893
		0.119	0.858	0.050	0.946
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.050	0.940	0.282	0.000	0.020	0.978	0.501	0.000
		0.073	0.914	0.356	0.006	0.030	0.968	0.573	0.025
		0.101	0.879	0.440	0.017	0.042	0.955	0.632	0.064
		0.151	0.820	0.513	0.035	0.066	0.929	0.657	0.117
		0.245	0.705	0.580	0.070	0.116	0.874	0.645	0.203
		0.410	0.480	0.581	0.193	0.240	0.734	0.495	0.429

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; $d = 0.78524$, $n = 1.3594$.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mode fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wooten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Nonane (*n*-nonane); C_9H_2O; [111-84-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018–23 (1966). [Eng. transl. Russ. J. Phys. Chem. **40**, 1619–20 (1966)].

Variables:

T/K$=$298

Compiled by:

A. Skrzecz

4.18. Ethanoll + Water + Nonane

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9929	0.000	0.999
		0.2218	0.7661	0.094	0.904
		0.2949	0.6881	0.133	0.864
		0.3677	0.6111	0.177	0.819
		0.4714	0.4952	0.253	0.740
		0.5307	0.4335	0.303	0.689
		0.5802	0.3777	0.352	0.638
		0.6201	0.3282	0.399	0.588
		0.6941	0.2483	0.493	0.491
		0.7504	0.1640	0.605	0.368
		0.7726	0.1262	0.664	0.302
		0.7699	0.0679	0.753	0.185
		0.7587	0.0516	0.777	0.147
		0.7354	0.0370	0.793	0.111
		0.7090	0.0274	0.798	0.086
		0.6533	0.0164	0.789	0.055
		0.6505	0.0160	0.788	0.054
		0.5122	0.0044	0.718	0.017
		0.4110	0.0016	0.637	0.007
		0.3409	0.0006	0.568	0.003

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.000	1.000	0.593	0.010	0.000	1.000	0.764	0.036
		0.064	0.936	0.681	0.021	0.024	0.976	0.796	0.068
		0.122	0.871	0.752	0.045	0.048	0.951	0.786	0.131
		0.265	0.723	0.775	0.114	0.116	0.882	0.682	0.280
		0.300	0.683	0.768	0.135	0.136	0.861	0.650	0.318
		0.377	0.597	0.745	0.177	0.184	0.811	0.588	0.388
		0.505	0.462	0.672	0.268	0.280	0.713	0.466	0.518
		0.521	0.442	0.665	0.279	0.295	0.697	0.454	0.531
		0.588	0.370	0.588	0.370	0.360	0.630	0.360	0.630

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, Ref. 1, was used to determine solubility of the mixtures. The third component was added to the binary homogenous mixture until cloudiness was first observed. Density of the saturated mixtures was measured; these results were graphed. To obtain equilibrium, ternary mixtures were stirred in a thermostated vessel for several hours. After phase separation, the density of each phase was measured and composition was determined from the graphs prepared earlier. Concentration at the critical point was found by method described in Ref. 2. Water included in ethanol was taken into account in all measurements.

Source and Purity of Materials:

(1) source not specified, ''rectificate grade;'' distilled; water concentration was determined by the Karl Fischer method.
(2) source not specified; b.p.$=$150.6 °C, n(25 °C,D)$=$1.4030.
(3) not specified.

Estimated Error:

solubility ±0.001 mass fraction.

References

[1] W. D. Bancroft, Phys. Rev. **3**, 21 (1896).
[2] E. N. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) 2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene (alpha-pinene, pinene); $C_{10}H_{16}$; [80-56-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

W. D. Bonner, J. Phys. Chem. **14**, 738–89 (1909–1910).

Variables:

T/K=273

Compiled by:

A. Skrzecz

4.19. Ethanol + Water + 2,6,6-Trimethylbicyclo [3.1.1] hept-2-ene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)	
0.0	273.2	0.4265	0.5328	0.2114	0.7808	
		0.5586	0.3958	0.3197	0.6701	plait point
		0.6851	0.2187	0.5002	0.4723	
		0.7378	0.1403	0.6146	0.3457	
		0.7409	0.0878	0.6940	0.2433	
		0.7219	0.0617	0.7300	0.1844	
		0.7065	0.0494	0.7452	0.1542	
		0.6818	0.0363	0.7582	0.1192	
		0.6497	0.0276	0.7576	0.0952	
		0.6144	0.0200	0.7524	0.0726	
		0.5682	0.0133	0.7368	0.0511	
		0.4981	0.0068	0.6998	0.0282	
		0.3980	0.0029	0.6211	0.0133	

Auxiliary Information

Method/Apparatus/Procedure:

In a tube 1 cm diameter and 12 cm long known amount, by weight, of hydrocarbon and water were placed into a temperature controlled bath. The contents of the tube were stirred and alcohol was added gradually until a homogeneous solution was obtained. Observations were made visually through the telescope of a cathetometer. The samples were always weighed immediately before and after each experiment. Concentrations were reported as weight of water in 1 g of binary water–hydrocarbon mixture and the weight of alcohol necessary to make a homogeneous solution. The mass of binary water–hydrocarbon mixture was about 1 g; the mass of alcohol—up to 5 g.

Source and Purity of Materials:

(1) Kahlbaum; presumably dried and distilled.
(2) Kahlbaum; presumably dried and distilled.
(3) not specified.

Estimated Error:

accuracy of weighing 0.0001 g.

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Decahydronaphthalene (cis+trans) (decalin, bicyclo[4.4.0]decane); $C_{10}H_{18}$; [91-17-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

F. Ruiz, V. Gomis, and R. F. Botella, Fluid Phase Equilib. **43**, 317–27 (1988).

Variables:

T/K=298

Compiled by:

A. Skrzecz

4.20. Ethanol + Water + Decahydronaphthalene (cis+trans)

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.7214	0.2448	0.491	0.500
		0.7826	0.1673	0.600	0.385
		0.7981	0.1224	0.667	0.307
		0.7990	0.0878	0.722	0.238
		0.7546	0.0481	0.773	0.148
		0.7076	0.0313	0.783	0.104
		0.5758	0.0100	0.750	0.039
		0.5181	0.0058	0.718	0.024

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.0009	0.9938	0.04244	0.0	0.0003	0.999	0.1018	0.0[a)]
		0.0051	0.9926	0.082032	0.000012	0.0017	0.998	0.186	0.00008
		0.0072	0.9928	0.121932	0.000034	0.0024	0.998	0.262	0.00022
		0.0104	0.9896	0.162777	0.000046	0.0035	0.997	0.332	0.00028
		0.0122	0.9878	0.204236	0.000125	0.0041	0.996	0.396	0.00073
		0.0136	0.9833	0.24807	0.00027	0.0046	0.995	0.457	0.0015
		0.0172	0.9813	0.29623	0.00059	0.0058	0.994	0.517	0.0031
		0.0181	0.9819	0.33748	0.00110	0.0061	0.994	0.563	0.0055
		0.0187	0.9813	0.38728	0.00187	0.0063	0.994	0.613	0.0089
		0.0195	0.9775	0.43963	0.00320	0.0066	0.993	0.659	0.0144
		0.0227	0.9750	0.48531	0.00487	0.0077	0.992	0.694	0.0209
		0.0262	0.9730	0.53337	0.00760	0.0089	0.991	0.725	0.0310
		0.0323	0.9677	0.59358	0.01172	0.0110	0.989	0.758	0.0449
		0.0366	0.9634	0.63462	0.01666	0.0125	0.988	0.773	0.0609

[a] No detectable composition of decalin.

Auxiliary Information

Method/Apparatus/Procedure:

The cloud point method was used to determine the solubility curve. The experimental apparatus was described in Ref. 1. The analytical method was used to determine liquid–liquid equilibria. Mixtures of known overall composition, by weight, were stirred intensely and allowed to settle for 2 h at constant temperature bath. Samples of each phase were taken and analyzed by glc method with 1-propanol as internal standard. (1-Propanol also prevented phase separation.) Analytical conditions: column 2 m×3 mm, packed with Chromosorb 101 100/120, temp. 190 °C, thermal conductivity detector for the organic phase, flame ionization detector for aqueous phase, helium flow rate −40mL/min. Water was reported to be undetectable in the organic phase.

Source and Purity of Materials:

(1) Merck; used as received; <0.2 wt % impurities by glc.
(2) Merck; used as received; mixture of cis- and trans-isomers.
(3) not reported.

Estimated Error:

temp. ±0.1 °C; relative accuracy of composition 2% (solubility curve).

References:

[1] F. Ruiz and D. Prats, Fluid Phase Equilib. **10**, 77 (1983).

Components:

(1) Ethanol (ethyl alcohol); C_2H_6O; [64-17-5]
(2) Decane (*n*-decane); $C_{10}H_{22}$; [124-18-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. V. Sadovnikova and M. V. Alexandrova, Sb. Nauch. Tr., Vladimir. Vech. Politekh. Inst. **12**, 137–9 (1971).

Variables:

T/K = 293

Compiled by:

A. Skrzecz

4.21. Ethanol + Water + Decane

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
20	293.2	0.0174	0.9811	0.0057	0.9941
		0.8781	0.1219	0.7000	0.3000
		0.8906	0.0884	0.7600	0.2330
		0.8902	0.0697	0.7940	0.1920
		0.8521	0.0350	0.8485	0.1075
		0.8135	0.0254	0.8520	0.0820
		0.7447	0.0133	0.8460	0.0465
		0.6472	0.0048	0.8110	0.0185
		0.4520	0.0005	0.6770	0.0023
		0.3501	0.00026	0.5787	0.0013
		0.2206	0.000034	0.4198	0.0002
		0.10189	0.000022	0.22485	0.00015

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20	293.2	0.0040	0.9952	0.5703	0.4287	0.00130	0.99860	0.30100	0.69881
		0.0089	0.9899	0.7348	0.2479	0.00290	0.99695	0.48750	0.50800
		0.0174	0.9811	0.8502	0.1399	0.00570	0.99410	0.66100	0.33600
		0.0299	0.9693	0.9033	0.0804	0.00990	0.99000	0.78000	0.21450
		0.0347	0.9653	0.8781	0.1219	0.0115	0.9885	0.6800	0.3200

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to obtain compositions along the saturation curve and the analytical method—for compositions of coexisting phases.

Source and Purity of Materials:

(1) source not specified; distilled on 20 TP column; n(20 °C,D) = 1.3627.
(2) source not specified; distilled on 20 TP column; n(20 °C,D) = 1.4119.
(3) distilled.

Estimated Error:

temp. ±0.1 °C.

5. 1-Propanol + Water

Components:

(1) 1-Proponal (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.02)

5.1. 1-Propanol + Water + Benzene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-propanol–benzene–water is given in Table 41.

TABLE 41. Summary of experimental data for the system 1-propanol–benzene–water

Author(s)	T/K	Type of data[a]	Ref.
Holmes, 1918	288	sat. (1)	1
Leikola, 1940	293	sat. (8)	2
Denzler, 1945	293	sat. (17), eq. (12)	3
McCants *et al.*, 1953	311	sat. (11), eq. (6)	4
Udovenko and Mazanko, 1963	288–352	sat. (87), eq. (38)	5
Letcher *et al.*, 1990	298	sat. (14), eq. (5)	6

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 1-propanol–benzene–water forms a miscibility gap of type 1. The miscibility gap was observed to increase with decreasing temperature. Only one binary system, benzene–water, forms a miscibility gap. These binary data were compiled and critically evaluated in a previously published SDS volume.[7] This critical evaluation is based on the original papers with the exception of data of Leikola,[2] which were taken from the handbook of Kafarov;[8] this data set was also taken into account during evaluation but is not reported as a compilation sheet because it does not contribute further to knowledge of the system. Data of Letcher *et al.*[6] were presented in the original paper only in graphical form and therefore are not reported as a compilation. Data of Udovenko and Mazanko[5] were reported at saturation temperatures of mixtures containing a constant ratio of two components. A large number of experimental points (87) was reported over the temperature range 288–352 K, but were not used for constant temperature data comparisons. In Ref. 3 one point in the organic-rich phase at 293 K, $x_1=0.4439$, is rejected since it has an unrealistically high amount of 1-propanol. The comparison of recommended binary data (Ref. 7) was possible only with experimental data of McCants *et al.*[4] at 310.9 K. The mutual solubility of the binary benzene–water system in Ref. 4 was reported to be $x_2'=0.9871$ and $x_2''=0.0012$, while the recommended values interpolated at this temperature by the evaluator on the basis of Ref. 7 are $x_2'=0.9954$ and $x_2''=0.000\,44$. Other references did not report information about the binary system. Equilibrium data, reported in Refs. 3, 4, and 5, were included in the evaluation of saturation the curve. All data are consistent within each data set as well as with one another. All are treated as tentative. Temperature of 293.2 K was selected and data of Leikola[2] and Denzler[3] were fitted to the equation:

$$x_1=a_1\cdot z_1\cdot \ln(z_1)+a_2\cdot z_2 \ln(z_2)+a_3\cdot z_1\cdot z_2 .$$

where: $z_1=(x_2+0.5\cdot x_1-x_{20}'')/(x_{20}'-x_{20}'')$, $z_2=(x_{20}'-x_2-0.5\cdot x_1)/(x_{20}'-x_{20}'')$, x_1, x_2-mole fractions of component (1) and (2) respectively, x_{20}', x_{20}''-values of x_2 on the saturation curve which cuts the $x_1=0$ axis.

The equation was proposed by Hlavaty[9] and also used with success by Letcher *et al.*[10] for the description of saturation curves of the ternary alcohol–ether–water systems. This equation gives better results (smaller standard deviation) for this system than any other tested equations. The parameters obtained by the least squares method for the whole range of saturation curve are: $a_1=-0.018\,96$, $a_2=0.462\,78$, $a_3=2.394\,28$. The standard error of estimate was 0.0094. For selected concentrations of benzene in the mixture, the saturation curve was calculated and the results are presented in Table 42 and in Fig. 21 as a solid line.

TABLE 42. Calculated compositions along the saturation curve at 293.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 406 Ref. 7	0.3571	0.5000
0.0490	0.0010	0.3453	0.5200
0.1612	0.0100	0.3331	0.5400
0.2190	0.0200	0.3204	0.5600
0.2898	0.0400	0.3074	0.5800
0.3353	0.0600	0.2939	0.6000
0.3676	0.0800	0.2802	0.6200
.03916	0.1000	0.2661	0.6400
0.4096	0.1200	0.2517	0.6600
0.4231	0.1400	0.2370	0.6800
0.4329	0.1600	0.2221	0.7000
0.4399	0.1800	0.2070	0.7200
0.4444	0.2000	0.1916	0.7400
0.4469	0.2200	0.1761	0.7600
0.4475	0.2400	0.1604	0.7800
0.4466	0.2600	0.1446	0.8000
0.4443	0.2800	0.1286	0.8200
0.4407	0.3000	0.1127	0.8400
0.4360	0.3200	0.0967	0.8600
0.4303	0.3400	0.0807	0.8800
0.4237	0.3600	0.0648	0.9000
0.4162	0.3800	0.0492	0.9200
0.4080	0.4000	0.0339	0.9400
0.3990	0.4200	0.0193	0.9600
0.3894	0.4400	0.0061	0.9800
0.3792	0.4600	0.0000	0.9975 Ref. 7
0.3684	0.4800		

Phase in equilibrium

The phases in equilibrium were measured at constant temperatures: 293 K (Ref. 3), 298 K (Ref. 6), 303 K (Ref. 5), 311 K (Ref. 4), 318 K and 333 K (Ref. 5). The tie lines cover the whole area of miscibility gap, all together 61 tie lines were reported. They are consistent within each data set, within each region as well as between regions. Letcher and Siswana on the basis previous experiments, Ref. 6, calculated the plait point in Ref. 11. Characteristic points on binodal curve, plait point and maximum 1-propanol concentration, reported or estimated, are presented at selected temperatures in Table 43. At maximum 1-propanol concentration the errors estimated by the evaluator are 0.005 and 0.02 mole fraction of 1-propanol and benzene, respectively.

TABLE 43. Characteristic points on the binodal curve of the system 1-propanol–benzene–water

	Max. C_3H_7OH concentration			Plait points		Ref.
T/K	x_1	x_2	Ref.	x_1	x_2	Ref.
288.2	0.438	0.198	3	0.173	0.014	3
293.2	0.458	0.220	3	—	—	
298.2	0.43	0.20	6	0.18	0.01	11
303.2	0.3917	0.101	5	0.172	0.014	5
310.9	0.396	0.151	4	—	—	
318.2	0.412	0.272	5	0.162	0.015	5
333.2	0.390	0.182	5	0.158	0.017	5

The plait point changes very slightly with temperature. The concentration of 1-propanol at the plait point increases very slowly with decreasing temperature [from $x_1=0.158$ at 333 K (Ref. 5) to $x_1=0.173$ at 293 K (Ref. 3)]; while the concentration of benzene is nearly independent of temperature (it varied from 0.017 to 0.014). The experimental tie lines at 293.2 K, Ref. 3, are presented in Fig. 21 together with the saturation curve as an example of the system property.

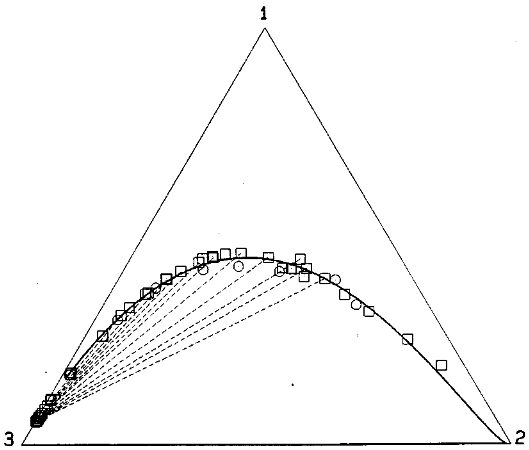

FIG. 21. Phase diagram of the system 1-propanol (1)—benzene (2)—water (3) at 293.2 K. ○—experimental results of Ref. 2, □—experimental results of Ref. 3, dashed lines—experimental tie lines, Ref. 3.

References:

[1] J. Holmes, J. Chem. Soc. **113**, 263 (1918).

[2] E. Leikola, Suom. Kemistil. B **13**, 13 (1940).

[3] C. G. Denzler, J. Phys. Chem. **49,** 358 (1945).

[4] J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454 (1953).

[5] V. V. Udovenko and T. F. Mazanko, Zh. Fiz. Khim. **37,** 1151 (1963).

[6] T. M. Letcher, J. Sewry, and S. Radloff, S. Afr. J. Chem. **43**, 56 (1990).

[7] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[8] V. V. Kafarov, ed., *Spravochnik po Rasivormosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskya, 1963).

[9] K. Hlavaty, Collect. Czech. Chem. Commun. **37**, 4005 (1972).

[10] T. M. Letcher, S. Ravindran, and S. E. Radloff, Fluid Phase Equilib, **69**, 251 (1991).

[11] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

C. G. Denzler, J. Phys. Chem. **49**, 358–65 (1945).

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
20.0	293.2	0.0671	0.0009	0.193	0.0035
		0.1103	0.0047	0.289	0.016
		0.1689	0.0140	0.391	0.042
		0.2622	0.0338	0.507	0.085
		0.3297	0.0550	0.563	0.122
		0.3605	0.0726	0.577	0.151
		0.3979	0.0960	0.590	0.185
		0.4447	0.1477	0.586	0.253
		0.4507	0.1644	0.578	0.274
		0.4562	0.1882	0.565	0.303
		0.4234	0.3222	0.461	0.456
		0.4221	0.3406	0.451	0.473
		0.4034	0.3760	0.421	0.510
		0.3606	0.4809	0.349	0.605
		0.3203	0.5507	0.298	0.666
		0.2531	0.6632	0.222	0.756
		0.1889	0.7633	0.158	0.830

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20.0	293.2	0.1732	0.0141	0.1732	0.0141	0.398	0.042	0.398	0.042[b]
		0.3109	0.0478	0.1068	0.0056	0.550	0.110	0.281	0.019[a]
		0.3646	0.0757	0.0937	0.0048	0.578	0.156	0.253	0.017
		0.3961	0.0988	0.0859	0.0039	0.586	0.190	0.236	0.014
		0.4148	0.1176	0.0754	0.0033	0.586	0.216	0.212	0.012[a]
		0.4360	0.1441	0.0704	0.0030	0.582	0.250	0.200	0.011[a]
		0.4472	0.1675	0.0671	0.0027	0.573	0.279	0.192	0.010
		0.4579	0.2198	0.0634	0.0024	0.545	0.340	0.183	0.009[a]
		0.4479	0.2806	0.0626	0.0021	0.501	0.408	0.181	0.008
		0.4439	0.3482	0.0590	0.0018	0.463	0.472	0.172	0.007
		0.4216	0.3720	0.0570	0.0016	0.436	0.500	0.167	0.006[a]
		0.3981	0.4217	0.0554	0.0010	0.398	0.548	0.163	0.004

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine the binodal curve. Binary mixtures of known mass and composition, by weight, were placed in a thermostat and were titrated with the third component, added from a burette, until the second liquid phase was observed. The mass of the titrant was determined gravimetrically. Refractive indexes were measured at 25 °C, to be sure that samples are clear, and plotted for each component of the system. To determine tie-line, the two-phase mixtures of known total composition were placed into a thermostat bath and when equilibrium was reached, the refractive index of the top layer was measured. The compositions were read from prepared previously plots. The composition of the other phase in equilibrium was calculated from the mass balance. From several tie lines determined experimentally, Bachman charts were constructed and more lines were added by interpolation (a). The plait point was determined by extrapolation of the lines on Bachman chart to intersect with the equilibrium curve (b).

Source and Purity of Materials:

(1) source not specified, chemically pure grade; dried over $CaCl_2$, distilled three times; $n(20\ °C) = 1.3860$.
(2) source not specified, chemically pure grade; used as received; $n(20\ °C) = 1.5010$.
(3) not specified; $n(20\ °C) = 1.3330$.

Estimated error:

temp. ±0.1 °C

Components:

(1) 1-Propanol, (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454–6 (1953).

Variables:

T/K = 311

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
100	310.9	0.0000	0.9871	0.000	0.997
		0.2811	0.5886	0.259	0.705
		0.3261	0.4570	0.331	0.603
		0.3917	0.3284	0.434	0.473
		0.3964	0.1514	0.544	0.270
		0.3673	0.1025	0.557	0.202
		0.2786	0.0471	0.514	0.113
		0.2246	0.0312	0.460	0.083
		0.1712	0.0192	0.390	0.057
		0.0870	0.0048	0.238	0.017
		0.0000	0.0012	0.000	0.005

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich-phase (compiler)		hydrocarbon-rich phase		water-rich phase	
100	310.9	0.0496	0.9377	0.0188	0.0007	0.039	0.958	0.060	0.003
		0.1119	0.8512	0.0252	0.0015	0.091	0.900	0.079	0.006a)
		0.1786	0.7658	0.0338	0.0018	0.150	0.836	0.104	0.007a)
		0.3278	0.4888	0.0469	0.0026	0.322	0.624	0.140	0.010a)
		0.3854	0.3458	0.0564	0.0026	0.421	0.491	0.165	0.010b)
		0.0990	0.8680	0.0290	0.0017	0.080	0.912	0.090	0.007b)

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to obtain binodal curve. The samples of homogenous binary mixture were placed in a constant temperature bath and titrated the third component to the cloud point. Each sample was agitated in the constant temperature bath for several minutes between drops of the third component. The temperatures of these systems were raised slightly (1 °F) to obtain homogeneity and their refractive indexes were measured. The analytical method was used for tie lines. (a) A ternary mixture of known composition was shaken for several hours in constant temperature bath and after both phases were carefully separated and their refractive indexes were determined. The intersections of the tie lines with the binodal curve were determined by refractive index interpolations between points of known composition used to determine the curve. (b) The slopes of the tie lines were checked by determining tie lines by the graphical application of the lever rule as described in Ref. 1.

Source and Purity of Materials:

(1) Du Pont, refined; used as received; $n(20\ °C,D) = 1.3855$, $d(75\ °F,60\ °F) = 0.800$.
(2) Baker, thiophene free; used as received; $n(20\ °C,D) = 1.5004$, $d(75\ °F,60\ °F) = 0.873$.
(3) distilled; $n(20\ °C,D) = 1.3330$.

Estimated Error:

refractive index ±0.0001; concentration ±0.001 mass % (estimated by compiler).

References:

[1] D. F. Othmer and P. E. Tobias, Ind. Eng. Chem. **34**, 690 (1942).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Benzene: C_6H_6; [71-43-2]
(3) Water; H_2O; [1732-18-5]

Original Measurements:

V. V. Udovenko and T. F Mazanko, Zh. Fiz. Khim. **37**, 1151–3 (1963). [Eng. transl. Russ. J. Phys. Chem. **37**, 610–2 (1963)].

Variables:

T/K = 288–352

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
16.75	289.90	0.1237	0.8519	0.0999	0.8942
27.62	300.77	0.1232	0.8484	0.0998	0.8933
39.45	312.60	0.1227	0.8452	0.0997	0.8925
51.50	324.65	0.1222	0.8418	0.0996	0.8916
60.62	333.77	0.1217	0.8379	0.0995	0.8906
70.57	343.72	0.1213	0.8359	0.0994	0.8901
21.00	294.15	0.2287	0.7059	0.1962	0.7870
25.75	298.90	0.2280	0.7033	0.1961	0.7862
26.42	299.57	0.2273	0.7014	0.1959	0.7857
41.63	314.78	0.2258	0.6964	0.1956	0.7842
47.50	320.65	0.2250	0.6940	0.1954	0.7835
59.50	332.65	0.2231	0.6883	0.1950	0.7818
68.01	341.16	0.2211	0.6822	0.1945	0.7800
16.22	289.37	0.3098	0.5683	0.2855	0.6808
25.60	298.75	0.3078	0.5647	0.2850	0.6796
33.73	306.88	0.3061	0.5615	0.2846	0.6785
47.77	320.92	0.3028	0.5555	0.2837	0.6765
57.60	330.75	0.3003	0.5507	0.2831	0.6748
69.73	342.88	0.2968	0.5445	0.2821	0.6727
17.25	290.40	0.3797	0.4261	0.3829	0.5584
27.50	300.65	0.3759	0.4218	0.3817	0.5567
38.27	311.42	0.3713	0.4166	0.3803	0.5546
44.75	317.90	0.3684	0.4133	0.3794	0.5532
54.60	327.75	0.3640	0.4083	0.3780	0.5511
58.59	331.74	0.3622	0.4063	0.3774	0.5503
63.25	336.40	0.3606	0.4045	0.3769	0.5495
73.40	346.55	0.3570	0.4005	0.3757	0.5478
18.11	291.26	0.4191	0.3140	0.4619	0.4499
33.50	306.65	0.4100	0.3072	0.4586	0.4466
40.49	313.64	0.4058	0.3040	0.4570	0.4450
54.02	327.17	0.3958	0.2965	0.4531	0.4413
60.50	333.65	0.3902	0.2923	0.4509	0.4391
67.53	340.68	0.3831	0.2871	0.4480	0.4364
14.70	287.85	0.4362	0.2523	0.5087	0.3824
26.67	299.82	0.4287	0.2480	0.5056	0.3801
33.65	306.80	0.4227	0.2444	0.5031	0.3781
46.98	320.13	0.4118	0.2381	0.4984	0.3746
54.87	328.02	0.4040	0.2336	0.4949	0.3720
64.12	337.27	0.3948	0.2284	0.4907	0.3689
78.60	351.75	0.3782	0.2187	0.4828	0.3629

19.12	292.27	0.4364	0.1828	0.5537	0.3015
23.38	296.53	0.4325	0.1811	0.5518	0.3004
30.27	303.42	0.4255	0.1782	0.5484	0.2985
45.63	318.78	0.4104	0.1718	0.5407	0.2943
55.58	328.73	0.2962	0.1241	0.4692	0.2555
63.95	337.10	0.3889	0.1629	0.5291	0.2881
76.25	349.40	0.3746	0.1569	0.5210	0.2837
18.90	292.05	0.4134	0.1150	0.5870	0.2122
32.78	305.93	0.3958	0.1101	0.5761	0.2083
46.35	319.50	0.3784	0.1052	0.5648	0.2041
53.83	326.98	0.3665	0.1019	0.5567	0.2012
61.87	335.02	0.3548	0.0986	0.5485	0.1982
71.60	344.75	0.3357	0.0934	0.5344	0.1932
20.00	293.15	0.3571	0.0696	0.5765	0.1461
37.75	310.90	0.3316	0.0647	0.5558	0.1409
50.49	323.64	0.3083	0.0601	0.5355	0.1357
63.00	336.15	0.2822	0.0550	0.5108	0.1295
69.09	342.24	0.2662	0.0519	0.4947	0.1254
28.38	301.53	0.0724	0.0019	0.2055	0.0070
41.88	315.03	0.0724	0.0025	0.2050	0.0092
48.35	321.50	0.0723	0.0030	0.2046	0.0109
65.52	338.67	0.0723	0.0038	0.2040	0.0141
73.32	346.47	0.0722	0.0046	0.2034	0.0170
20.25	293.40	0.1131	0.0051	0.2945	0.0174
33.23	306.38	0.1130	0.0062	0.2935	0.0208
41.00	314.15	0.1129	0.0070	0.2927	0.0235
56.45	329.60	0.1127	0.0086	0.2911	0.0288
67.95	341.10	0.1125	0.0102	0.2895	0.0340
21.08	294.23	0.1668	0.0121	0.3891	0.0367
32.35	305.50	0.1666	0.0135	0.3875	0.0407
46.12	319.27	0.1662	0.0154	0.3851	0.0465
53.61	326.76	0.1660	0.0164	0.3839	0.0494
65.40	338.55	0.1656	0.0193	0.3806	0.0577
73.81	346.96	0.1653	0.0210	0.3786	0.0626
18.12	291.27	0.2217	0.0217	0.4651	0.0592
23.50	296.65	0.2216	0.0225	0.4641	0.0612
35.48	308.63	0.2212	0.0245	0.4616	0.0664
50.71	323.86	0.2204	0.0277	0.4574	0.0748
62.30	335.45	0.2197	0.0310	0.4533	0.0832
70.15	343.30	0.2190	0.0339	0.4497	0.0904
18.45	291.60	0.2993	0.0390	0.5458	0.0924
28.80	301.95	0.2984	0.0419	0.5419	0.0989
37.67	310.82	0.2975	0.0447	0.5381	0.1052
48.20	321.35	0.2963	0.0487	0.5330	0.1138
61.25	334.40	0.2943	0.0549	0.5249	0.1272
69.28	342.43	0.2927	0.0603	0.5180	0.1387

		Compositions of coexisting phases							
		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/°C$	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
30	303.2	0.0168	0.9789	0.0108	0.0002	0.0130	0.9860	0.0350	0.0010
		0.0447	0.9467	0.0214	0.0004	0.0350	0.9630	0.0680	0.0015
		0.1181	0.8611	0.0330	0.0005	0.0950	0.9000	0.1020	0.0020
		0.2119	0.7292	0.0372	0.0008	0.1800	0.8050	0.1140	0.0030
		0.3217	0.5366	0.0412	0.0009	0.3030	0.6570	0.1250	0.0035
		0.3754	0.3999	0.0448	0.0010	0.3900	0.5400	0.1350	0.0040
		0.4143	0.2916	0.0475	0.0012	0.4700	0.4300	0.1420	0.0045
		0.4279	0.1814	0.0539	0.0013	0.5480	0.3020	0.1590	0.0050
		0.3917	0.1013	0.0625	0.0019	0.5800	0.1950	0.1810	0.0070
		0.3576	0.0718	0.0744	0.0025	0.5750	0.1500	0.2100	0.0090
		0.3337	0.0593	0.0753	0.0027	0.5630	0.1300	0.2120	0.0100
		0.2979	0.0433	0.0953	0.0043	0.5400	0.1020	0.2570	0.0150
		0.1721	0.0144	0.1721	0.0144	0.3960	0.0430	0.3960	0.0430[a]
45	318.2	0.0090	0.9866	0.0083	0.0005	0.0070	0.9920	0.0270	0.0020
		0.0269	0.9645	0.0205	0.0007	0.0210	0.9770	0.0650	0.0030
		0.1353	0.8241	0.0296	0.0010	0.1110	0.8790	0.0920	0.0040
		0.2226	0.7039	0.0334	0.0012	0.1920	0.7890	0.1030	0.0050
		0.3169	0.5382	0.0370	0.0015	0.2990	0.6600	0.1130	0.0060
		0.3675	0.4073	0.0413	0.0018	0.3810	0.5490	0.1250	0.0070
		0.4122	0.2721	0.0435	0.0020	0.4790	0.4110	0.1310	0.0080
		0.4090	0.1602	0.0510	0.0023	0.5480	0.2790	0.1510	0.0090
		0.3576	0.0839	0.0619	0.0029	0.5640	0.1720	0.1790	0.0110
		0.3070	0.0538	0.0786	0.0041	0.5400	0.1230	0.2190	0.0150
		0.2434	0.0317	0.1118	0.0074	0.4850	0.0820	0.2900	0.0250
		0.1623	0.0148	0.1623	0.0148	0.3790	0.0450	0.3790	0.0450[a]
60	333.2	0.0253	0.9453	0.0092	0.0002	0.0200	0.9730	0.0300	0.0010
		0.0562	0.9104	0.0140	0.0005	0.0450	0.9470	0.0450	0.0020
		0.1462	0.7864	0.0238	0.0010	0.1230	0.8600	0.0750	0.0040
		0.2370	0.6684	0.0285	0.0010	0.2090	0.7660	0.0890	0.0040
		0.3075	0.5379	0.0324	0.0012	0.2920	0.6640	0.1000	0.0050
		0.3612	0.3928	0.0388	0.0020	0.3820	0.5400	0.1180	0.0080
		0.3859	0.3070	0.0436	0.0023	0.4400	0.4550	0.1310	0.0090
		0.3902	0.1818	0.0514	0.0026	0.5170	0.3130	0.1520	0.0100
		0.3582	0.1019	0.0653	0.0035	0.5490	0.2030	0.1870	0.0130
		0.3394	0.0842	0.0707	0.0041	0.5460	0.1760	0.2000	0.0150
		0.2998	0.0581	0.0780	0.0050	0.5280	0.1330	0.2170	0.0180
		0.2315	0.0327	0.1035	0.0082	0.4680	0.0860	0.2720	0.0280
		0.1581	0.0168	0.1581	0.0168	0.3700	0.0510	0.3700	0.0510[a]

[a]Critical point of solubility.

Auxiliary Information

Method/Apparatus/Procedure:

Solubility was measured by Alekseev's method.[1] Nine solubility–temperature curves of constant alcohol–benzene ratio and another five curves of constant alcohol–water ratio were constructed. The method of phase equilibrium measurements was not reported. Critical points of solubility were obtained by Bachman,[2] and Alekseev's[1] methods.

Source and Purity of Materials:

(1) source not specified; purified; b.p.=96.5 °C at 750 Torr, $d(30\ °C,4\ °C)=0.7956$, $n(25\ °C,D)=1.3837$.
(2) source not specified; purified; b.p.=79.0 °C, at 752.5 Torr, $d(30\ °C,4\ °C)=0.8680$, $n(25\ °C,D)=1.4980$.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Gornyi Zh. **4**, 83 (1897).
[2] J. Bachman, Ind. Eng. Chem. Anal. Ed. **2**, 38 (1940).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz (Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.04)

5.2. 1-Propanol + Water + Cyclohexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-propanol–cyclohexane–water is given in Table 44.

TABLE 44. Summary of experimental data for the system 1-propanol–cyclohexane–water

Author(s)	T/K	Type of data[a]	Ref.
Washburn *et al.*, 1942	298, 308	sat. (32), eq. (18)	1
Letcher *et al.*, 1991	298	sat. (15), eq. (5)	2
Plackov and Stern, 1992	298	sat. (20), eq. (5)	3

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 1-propanol–cyclohexane–water forms a miscibility gap of type 1 covering the majority of the concentration triangle. Studies of the system were reported in three references at 298.2 K. Only Washburn *et al.*[1] also investigated this system at 308.2 K. All saturation data are consistent. Only the cyclohexane–water binary system forms a miscibility gap. The data for this binary system were compiled and critically evaluated in a previously published SDS volume;[4] the recommended values at 298.2 K are: $x_2''=1.2\cdot 10^{-5}$ and $x_3'=3.7\cdot 10^{-4}$. The end points of the saturation curve, Ref. 2, were reported to be $x_2=0.998$ and pure water which is not consistent with recommended values. However, these results are within the accuracy of experimental measurements (0.005 mole fraction) stated by the authors. One experimental point in the water-rich phase[3] was reported to be $x_1=0.053$, $x_2=0.000$, which may suggest that 1-propanol is only partially soluble in water. This numerical result reflects a lack of sensitivity of the analytical method used for cyclohexane in the water-rich phase. All experimental solubility and equilibrium data reported at 298.2 K in Refs. 1, 2, and 3, were used to construct the equation:

$$x_1=a_1\cdot(\ln z_1)^{a_2}\cdot z_1{}^{a_3}.$$

where: $z_1=(x_2+0.5\cdot x_1-x_{20}'')/(x_{20}'-x_{20}'')$, x_1,x_2—mole fractions of component (1) and (2), respectively, x_{20}',x_{20}''—values of x_2 on the binodal curve which cuts the $x_1=0$ axis. This equation has been proposed by Letcher *et al.*[5] for the description of saturation curves of the ternary alcohol–ether–water systems. It gives better results (the smallest standard deviation) for the investigated system than any other tested equation. The parameters obtained by the least squares method for the whole range of miscibility gap (water-rich and hydrocarbon-rich branches were described together) are: $a_1=1.50825$, $a_2=0.98056$, $a_3=1.28405$. The standard error of estimate was 0.0084. For selected concentrations of cyclohexane in the mixture, saturation curve was calculated by the above equation. The results are presented in the Table 45 and in Fig. 22 as solid line.

TABLE 45. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 012 Ref. 4	0.3607	0.5000
0.0288	0.0010	0.3504	0.5200
0.1697	0.0100	0.3397	0.5400
0.2233	0.0200	0.3285	0.5600
0.2870	0.0400	0.3169	0.5800
0.3279	0.0600	0.3049	0.6000
0.3572	0.0800	0.2925	0.6200
0.3791	0.1000	0.2797	0.6400
0.3958	0.1200	0.2666	0.6600
0.4085	0.1400	0.2531	0.6800
0.4181	0.1600	0.2394	0.7000
0.4251	0.1800	0.2253	0.7200

0.4299	0.2000	0.2109	0.7400
0.4328	0.2200	0.1963	0.7600
0.4342	0.2400	0.1813	0.7800
0.4341	0.2600	0.1661	0.8000
0.4327	0.2800	0.1506	0.8200
0.4303	0.3000	0.1349	0.8400
0.4267	0.3200	0.1189	0.8600
0.4223	0.3400	0.1026	0.8800
0.4170	0.3600	0.0861	0.9000
0.4109	0.3800	0.0694	0.9200
0.4041	0.4000	0.0524	0.9400
0.3966	0.4200	0.0352	0.9600
0.3885	0.4400	0.0176	0.9800
0.3798	0.4600	0.0088	0.9900
0.3705	0.4800	0.0000	0.999 63 Ref. 4

Phases in equilibrium

Compositions of coexisting phases in the ternary system 1-propanol–cyclohexane–water at equilibrium were reported in all three references at 298.2 and at 308.2 K (Ref. 1). The tie lines cover the full area of the miscibility gap. The reported equilibrium data sets are not always consistent with one another, although they are consistent within each data set. Inconsistency is observed at the region near the plait point (the water-rich phase in equilibrium with the organic phase containing more than 0.25 mole fraction of alcohol). The data for phases in equilibrium are considered tentative. All experimental tie lines as well as experimental points, Refs. 1, 2, and 3 at 298.2 K, are shown in Fig. 22.

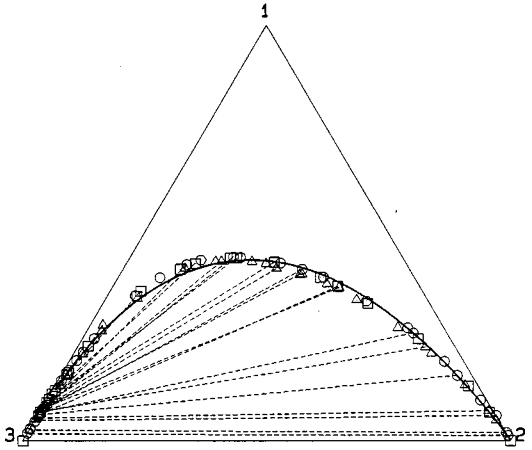

FIG. 22. Phase diagram of the system 1-propanol (1)—cyclohexane (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 1, □—experimental data, Ref. 2, △—experimental data, Ref. 3.

References:

[1] E. R. Washburn, C. E. Brockway, C. L. Graham, and P. Deming, J. Am. Chem. Soc. **64**, 1886 (1942).

[2] T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118 (1991).

[3] D. Plackov and I. Stern, Fluid Phase Equilib. **71**, 189 (1992).

[4] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[5] T. M. Letcher, S. Ravindran, and S. E. Radloff, Fluid Phase Equilib. **69**, 251 (1991).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. R. Washburn, C. E. Brockway, C. L. Graham, and P. Deming, J. Am. Chem. Soc. **64**, 1886–8 (1942).

Variables:

T/K=298–308

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.0983	0.8887	0.0730	0.9241
		0.1917	0.7686	0.1498	0.8409
		0.2727	0.6527	0.2255	0.7560
		0.3361	0.5362	0.2987	0.6673
		0.3933	0.4193	0.3794	0.5664
		0.4272	0.3141	0.4522	0.4657
		0.4410	0.2251	0.5150	0.3681
		0.4342	0.1474	0.5668	0.2695
		0.3920	0.0847	0.5873	0.1777
		0.3487	0.0558	0.5760	0.1291
		0.2467	0.0233	0.4952	0.0656
		0.1939	0.0138	0.4301	0.0429
		0.1456	0.0063	0.3563	0.0216
		0.1024	0.0019	0.2742	0.0072
		0.0637	0.0002	0.1849	0.0008
		0.0302	0.0001	0.0940	0.0006
35.0	308.2	0.1024	0.8833	0.0762	0.9206
		0.1903	0.7700	0.1486	0.8421
		0.2725	0.6525	0.2254	0.7560
		0.3380	0.5428	0.2981	0.6704
		0.3911	0.4269	0.3748	0.5729
		0.4278	0.3140	0.4527	0.4654
		0.4442	0.2303	0.5140	0.3731
		0.4343	0.1475	0.5668	0.2696
		0.3963	0.0867	0.5891	0.1805
		0.3543	0.0573	0.5799	0.1314
		0.2665	0.0274	0.5160	0.0742
		0.1933	0.0135	0.4296	0.0419
		0.1416	0.0064	0.3487	0.0221
		0.1028	0.0023	0.2746	0.0085
		0.0634	0.0003	0.1840	0.0011
		0.0295	0.0002	0.0921	0.0007

Compositions of coexisting phases

$t/°\mathrm{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hyrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.0126	0.9874	0.0181	0.0002	0.009	0.991	0.058	0.001
		0.0195	0.9805	0.0275	0.0007	0.014	0.986	0.086	0.003
		0.0606	0.9394	0.0464	0.0012	0.044	0.956	0.139	0.005
		0.1578	0.8118	0.0601	0.0015	0.121	0.872	0.175	0.006
		0.2599	0.6709	0.0674	0.0020	0.213	0.770	0.193	0.008
		0.4124	0.3660	0.0735	0.0018	0.416	0.517	0.208	0.007
		0.4422	0.2101	0.0781	0.0020	0.526	0.350	0.219	0.008
		0.4236	0.1240	0.0830	0.0028	0.578	0.237	0.230	0.011
		0.2141	0.0171	0.1702	0.0098	0.457	0.051	0.396	0.032
35.0	308.2	0.0153	0.9847	0.0194	0.0002	0.011	0.989	0.062	0.001
		0.0249	0.9704	0.0264	0.0002	0.018	0.981	0.083	0.001
		0.0907	0.9002	0.0440	0.0002	0.067	0.931	0.133	0.001
		0.1819	0.7837	0.0544	0.0002	0.141	0.851	0.161	0.001
		0.2956	0.6137	0.0606	0.0002	0.250	0.727	0.177	0.001
		0.4201	0.3563	0.0657	0.0000	0.426	0.506	0.190	0.000
		0.4437	0.1974	0.0710	0.0002	0.536	0.334	0.203	0.001
		0.4145	0.1066	0.0794	0.0008	0.586	0.211	0.223	0.003
		0.2318	0.0190	0.1502	0.0071	0.480	0.055	0.364	0.024

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, Refs 1,2, was used. Binary mixtures of known composition were titrated with the third component. The total weight of liquids employed was 13–15 g. The refractive indexes of mixtures were used to construct the refractive index/composition curve, which was used further to find compositions of equilibrium phases.

Source and Purity of Materials:

(1) Eastman Kodak Company, best grade; dried with active lime, distilled; $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.8000$, $n(25\ °\mathrm{C,D})=1.3838$.
(2) Eastman Kodak Company; distilled, dried with Na, recrystallized several times; $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.7746$, $n(25\ °\mathrm{C,D})=1.4232$, f.p. $=6.1\ °\mathrm{C}$.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] R. Vold and E. R. Washburn, J. Am. Chem. Soc. **54**, 4217 (1932).
[2] E. R. Washburn and H. C. Spencer, J. Am. Chem. Soc. **56**, 361 (1934).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118-21 (1991)

Variables:

$T/\mathrm{K}=298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°\mathrm{C}$ (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.070	0.001	0.200	0.004
		0.113	0.004	0.295	0.015
		0.165	0.011	0.386	0.036
		0.229	0.020	0.475	0.058
		0.347	0.060	0.570	0.138
		0.412	0.116	0.575	0.227
		0.440	0.205	0.528	0.344
		0.430	0.300	0.462	0.451
		0.393	0.413	0.382	0.562
		0.330	0.542	0.293	0.673
		0.246	0.688	0.200	0.784
		0.132	0.847	0.100	0.896
		0.068	0.922	0.050	0.948
		0.000	0.999	0.0000	0.9998

Compositions of coexisting phases

$t/°\mathrm{C}$ (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hyrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.371	0.460	0.061	0.001	0.348	0.604	0.178	0.004
		0.429	0.300	0.092	0.003	0.461	0.452	0.250	0.011
		0.440	0.218	0.100	0.004	0.519	0.360	0.267	0.015
		0.426	0.140	0.121	0.006	0.566	0.261	0.309	0.021
		0.360	0.062	0.160	0.010	0.581	0.140	0.378	0.033

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the titration method, as described in Ref. 1. The formation of a cloudy mixture was observed visually on shaking after addition of a known mass of the third component; syringes were precisely weighed. Tie line compositions were determined by the refractive index method, Ref. 2, and a complementary method using the Karl Fischer titration, Ref. 3. Measurements were made at pressure of 94.7 kPa.

Source and Purity of Materials:

(1) Merck; AR grade; refluxed with Mg and I_2, distilled; purity >99.9 mole % by glc.
(2) BDH; Gold label grade; used as received; purity >99.9 mole % by glc.
(3) not specified.

Estimated Error:

composition ±0.005 mole fraction (binodal curve), ±0.01 mole fraction (tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. Plackov and I. Stern, Fluid Phase Equilib. **71**, 189-209 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.0489	0.9452	0.0356	0.9631
		0.1347	0.8391	0.1022	0.8918
		0.2111	0.7319	0.1685	0.8179
		0.2732	0.6324	0.2301	0.7460
		0.3389	0.5149	0.3070	0.6533
		0.3767	0.4345	0.3616	0.5841
		0.4005	0.3716	0.4049	0.5261
		0.4257	0.2848	0.4671	0.4377
		0.4308	0.2540	0.4890	0.4038
		0.4315	0.1790	0.5401	0.3138
		0.4144	0.1251	0.5695	0.2408
		0.2647	0.0296	0.5113	0.0801
		0.2102	0.0174	0.4510	0.0523
		0.1588	0.0091	0.3772	0.0303
		0.1260	0.0043	0.3208	0.0153
		0.1041	0.0022	0.2775	0.0082
		0.0859	0.0010	0.2379	0.0039
		0.0702	0.0006	0.2008	0.0024
		0.0520	0.0004	0.1545	0.0017
		0.0254	0.0002	0.0799	0.0009

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hyrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25	298.2	0.072	0.918	0.053	0.000	0.053	0.945	0.157	0.000
		0.226	0.712	0.070	0.002	0.182	0.803	0.199	0.008
		0.368	0.464	0.077	0.003	0.345	0.608	0.216	0.012
		0.400	0.367	0.078	0.003	0.407	0.522	0.218	0.012
		0.414	0.312	0.079	0.003	0.444	0.468	0.220	0.012
		0.431	0.191	0.084	0.004	0.531	0.329	0.231	0.015
		0.279	0.025	0.134	0.010	0.534	0.067	0.331	0.035

Auxiliary Information

Method/Apparatus/Procedure:

Binodal compositions were determined by titration with the corresponding, less-soluble component until the appearance of turbidity.[1] The analytical method was used for determination of tie-lines. This was based on refractive indexes and densities of the samples,[1] combined with the oxidation of the alcohol with an excess of potassium dichromate and determination of unreduced dichromate with $Na_2S_2O_3$. Alcohol in the organic layer was determined after extraction with water.

Source and Purity of Materials:

(1) Kemika (Zagreb); analytical grade; presumably used as received; $n=1.3828$, $\rho(25\ °C)=799.6\ kg/m^3$, b.p. $=96.8\ °C$.
(2) Zorka (Sabac); purity not specified; presumably used as received; $n=1.4232$, $\rho(25\ °C)=773.6\ kg/m^3$, b.p. $=80.1\ °C$.
(3) twice distilled in the presence of $KMnO_4$.

Estimated Error:

composition <0.0005 mass fraction, binodal, (relative); composition $\pm 2\%$, tie line.

References:

[1] D. Plackov and I. Stern, Fluid Phase Equilib. **57**, 327 (1990).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland, (1994.11)

5.3. 1-Propanol + Water + Hexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-propanol–hexane–water is given in Table 46.

TABLE 46. Summary of experimental data for the system 1-propanol–hexane–water

Author(s)	T/K	Type of data[a]	Ref.
McCants *et al.*, 1953	311	sat. (16), eq. (5)	1
Vorobeva and Karapetyants, 1967	298	sat. (15), eq. (12)	2
Koshelkov *et al.*, 1974	334	eq. (5)	3
Sugi and Katayama, 1977	298	sat. (22), eq. (5)	4

[a] Number of experimental points in parentheses.

Saturation curve

The system 1-propanol–hexane–water forms miscibility gap of type 1. Only one binary system, hexane–water, is partially miscible. The data for this binary system were compiled and critically evaluated in previously published SDS volume.[5] The recommended values of mutual solubility of the hexane–water system at 298.2 K are: $x_2'=0.999\ 53$ and $x_2''=2.3\cdot 10^{-6}$. References 1, 2, and 4 also contain mutual solubility data for the binary system. Solubility of water in hexane ($x_2'=0.999\ 49$) reported by Sugi and Katayama[4] is consistent with recommended value of Ref. 5, while the results of McCants *et al.*,[1] at 310.9 K, and Vorobeva and Karapetyants[2] at 298.2 K differ significantly because they were measured with an accuracy of 0.001 wt. fraction and therefore are not able to describe properly mutual solubility in the binary system. Composition along the saturation curve were obtained by titration. Data for 298.2 K by Vorobeva and Karapetyants,[2] by Sugi and Katayama,[4] and for 310.9 K by McCants *et al.*[1], are consistent. The miscibility gap built on the basis of McCants *et al.* data[1] at 310.9 K is a little smaller, as is expected, than that for 298.2 K. Equilibrium data of Koshelkov *et al.*[3] at 334 K were reported at the boiling temperatures and are not entirely consistent with one another. The temperature 298.2 K was selected to present phase behavior. These data were used to construct the equation:

$$x_1=0.574\ 85+0.125\ 13\ \ln(x_3)+0.217\ 41x_3-0.821\ 37x_3^2.$$

The standard error of estimate was 0.0084. The equation is valid in the region of $0.001<x_3<0.83$. The compositions on the saturation curve calculated by the proposed equation are presented in Table 47 for selected concentrations of water in the mixture. The results of calculations (solid line) are also presented graphically in Fig. 23 together with all experimental data reported at 298.2 K.

TABLE 47. Calculated compositions along the saturation curve at 298.2 K

x_1	x_3	x_1	x_3
0.0000	0.000 47 Ref. 5	0.4127	0.4200
0.0893	0.0200	0.4088	0.4400
0.1794	0.0400	0.4039	0.4600
0.2329	0.0600	0.3981	0.4800
0.2709	0.0800	0.3915	0.5000
0.3002	0.1000	0.3756	0.5400
0.3238	0.1200	0.3665	0.5600
0.3432	0.1400	0.3565	0.5800
0.3593	0.1600	0.3457	0.6000
0.3728	0.1800	0.3341	0.6200
0.3841	0.2000	0.3217	0.6400
0.3935	0.2200	0.3086	0.6600
0.4011	0.2400	0.2946	0.6800

0.4073	0.2600	0.2799	0.7000
0.4120	0.2800	0.2645	0.7200
0.4155	0.3000	0.2483	0.7400
0.4177	0.3200	0.2313	0.7600
0.4188	0.3400	0.2136	0.7800
0.4188	0.3600	0.1952	0.8000
0.4178	0.3800	0.1760	0.8200
0.4157	0.4000	0.0000	0.999 997 7 Ref. 5

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 1-propanol–hexane–water are reported in four references. Data of Koshelkov *et al.*[3] were measured at boiling temperatures which were estimated by the compiler to be 334±1 K. In all cases similar procedures were used. When the equilibrium was reached, phases were separated and the composition of each phase was analyzed. The tie lines cover the whole range of miscibility gap. Data reported at 298.2 K by Vorobeva and Karapetyants[2] and by Sugi and Katayama[4] are in agreement with the exception of the range $x_3=0.88-0.90$ in the water-rich phase, where experimental equilibrium data are inconsistent, presumably due to the change of tie lines direction. The plait point of the system was reported only in Ref. 2 and is $x_1=0.214$, $x_2=0.017$. As with the saturation data, equilibrium data of McCants *et al.*[1] are reported at 310.9 K, a slightly higher temperature than in Refs. 2,4. The direction of tie lines at boiling temperatures, Ref. 3, is quite different than those at lower temperatures 298, 311 K, Refs. 1,2,4, but these data are consistent with those measured at boiling temperatures for the system 1-propanol–nonane–water, Ref. 3.

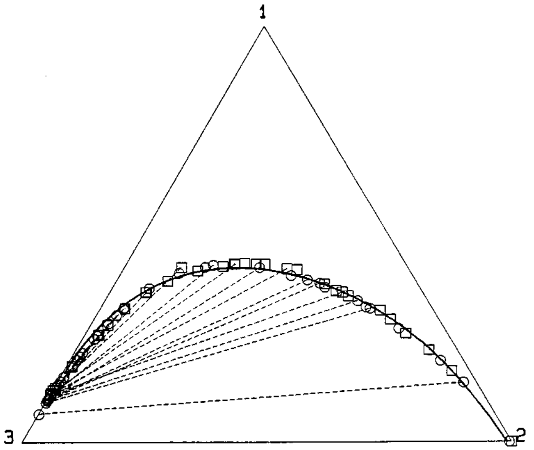

FIG. 23. Phase diagram of the system 1-propanol (1)—hexane (2)—water (3) at 298.2 K. Solid line—calculated binodal curve, ○—experimental results of Ref. 2, □—experimental results of Ref. 4, dashed lines—experimental tie lines, Refs. 2 and 4.

References:

[1] J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454 (1953).

[2] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144 (1967).

[3] V. A. Koshelkov, T. G. Pavlenko, V. N. Titova, V. S. Timofeev, and L. A. Serafimov, Tr. Altai. Politekh. Inst. im, I. I. Polzunova **41**, 84 (1974).

[4] H. Sugi and T. Katayama, J. Chem. Eng. Jpn. **10**, 400 (1977).

[5] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:	**Original Measurements:**
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8] (2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3] (3) Water; H_2O; [7732-18-5]	J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454-6 (1953).
Variables:	**Compiled by:**
T/K=311	A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°F	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
100	310.9	0.0000	0.9952	0.000	0.999
		0.2240	0.7008	0.179	0.803
		0.3083	0.5410	0.273	0.687
		0.3652	0.4382	0.347	0.597
		0.3984	0.3635	0.402	0.526
		0.4200	0.2815	0.460	0.442
		0.4229	0.1729	0.534	0.313
		0.4191	0.1322	0.564	0.255
		0.3881	0.0964	0.570	0.203
		0.3303	0.0546	0.557	0.132
		0.2352	0.0226	0.480	0.066
		0.1911	0.0161	0.423	0.051
		0.1439	0.0063	0.353	0.022
		0.0569	0.0010	0.167	0.004
		0.0292	0.0004	0.091	0.002
		0.0000	0.0002	0.000	0.001

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°F	T/K (compiler)	hyrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
100	310.9	0.0621	0.9148	0.0459	0.0007	0.045	0.950	0.138	0.003
		0.2237	0.6934	0.0729	0.0012	0.180	0.800	0.207	$0.005^{a)}$
		0.4228	0.2369	0.0929	0.0008	0.489	0.393	0.254	$0.003^{b)}$
		0.4218	0.1705	0.1054	0.0026	0.535	0.310	0.280	$0.010^{a)}$
		0.3773	0.4043	0.0879	0.0018	0.369	0.567	0.242	$0.007^{c)}$

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to obtain binodal curve. The samples of homogenous binary mixture were placed in a constant temperature bath and titrated the third component to the cloud point. Each sample was agitated in the constant temperature bath for several minutes between drops of the third component. The temperatures of these systems were raised slightly (1 °F) to obtain homogeneity and their refractive indexes were measured. The analytical method was used for tie lines.

(a) A ternary mixture of known composition was shaken for several hours in constant temperature bath and after both phases were carefully separated and their refractive indexes were determined. The intersections of the tie lines with the binodal curve were determined by refractive index interpolations between points of known composition used to determine the curve.

(b) The slopes of the tie lines were checked by determining tie lines by the graphical application of the lever rule as described in Ref. 1.

(c) The two phases were analyzed chemically for one or two components.

Source and Purity of Materials:

(1) Du Pont, refined; used as received; $n(20\ °\mathrm{C,D})=1.3855$, $d(75\ °\mathrm{F},60\ °\mathrm{F})=0.800$.

(2) Philips, pure grade; used as received; $n(20\ °\mathrm{C,D})=1.3752$, $d(75\ °\mathrm{F},60\ °\mathrm{F})=0.654$.

(3) distilled; $n(20\ °\mathrm{C,D})=1.3330$.

Estimated Error:

refractive index ±0.0001; concentration ±0.001 mass % (estimated by compiler).

References:

[1] D. F. Othmer and P. E. Tobias, Ind. Eng. Chem. **34**, 690 (1942).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144-9 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 602–5 (1967)].

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9952	0.000	0.999
		0.1422	0.8309	0.106	0.888
		0.1944	0.7581	0.150	0.839
		0.2724	0.6348	0.225	0.752
		0.3243	0.5423	0.284	0.681
		0.3719	0.4349	0.353	0.592
		0.4003	0.3515	0.409	0.515
		0.4204	0.1651	0.538	0.303
		0.4063	0.1188	0.565	0.237
		0.3699	0.0755	0.574	0.168
		0.3237	0.0473	0.558	0.117
		0.2564	0.0259	0.504	0.073
		0.2060	0.0148	0.447	0.046
		0.1978	0.0136	0.436	0.043
		0.1354	0.0042	0.339	0.015

Compositions of coexisting phases

		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
25	298.2	0.1422	0.8309	0.0678	0.0005	0.106	0.888	0.195	0.002
		0.3211	0.5522	0.0949	0.0015	0.279	0.688	0.258	0.006
		0.3397	0.5177	0.1000	0.0018	0.302	0.660	0.269	0.007
		0.3818	0.4198	0.1023	0.0018	0.366	0.577	0.274	0.007
		0.3898	0.3901	0.1052	0.0021	0.384	0.551	0.280	0.008
		0.4196	0.2774	0.1062	0.0021	0.462	0.438	0.282	0.008
		0.4253	0.1793	0.1115	0.0024	0.531	0.321	0.293	0.009
		0.3207	0.0471	0.1399	0.0048	0.555	0.117	0.347	0.017
		0.3057	0.0406	0.1463	0.0057	0.546	0.104	0.358	0.020
		0.2858	0.0338	0.1570	0.0070	0.531	0.090	0.376	0.024
		0.2483	0.0237	0.1833	0.0111	0.496	0.068	0.416	0.036
		0.2142	0.0167	0.2142	0.0167	0.457	0.051	0.457	0.051[a]

[a] Critical solubility point at 298.2 K.

Auxiliary Information

Method/Apparatus/Procedure:

The methods were reported in Ref. 1. The titration method was used to describe solubility of the mixtures. The third component was added to the binary homogeneous mixture until the cloudiness started to be observed. Density of the saturated mixtures was measured and put on the graphs. To obtain equilibrium ternary mixtures were stirred in thermostated vessel through several hours. After phase separation, density of each phase was measured and composition was determined from earlier prepared graphs. Concentration at critical point was found by the method described in Ref. 2. Water include in propanol was taken into account in all measurements.

Source and Purity of Materials:

(1) source not specified, chemical pure grade; distilled; water concentration was determined by the Karl Fischer method.
(2) source not specified; properties were the same as reported in Ref. 1.
(3) doubly distilled.

Estimated Error:
Not reported.

References:
[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[2] E. N. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:
(1)1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
V. A. Koshelkov, T. G. Pavlenko, V. N. Titova, V. S. Timofeev, and L. A. Serafimov, Tr. Altai. Politekh. Inst. im. I. I. Polzunova **41**, 84–92 (1994).

Variables:
$T/\mathrm{K}=334$

Compiled by:
A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/°\mathrm{C}$	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase complier		water-rich phase complier	
61	334	0.087	0.902	0.123	0.011	0.063	0.935	0.309	0.040
		0.122	0.833	0.169	0.036	0.093	0.898	0.368	0.112
		0.202	0.743	0.262	0.098	0.157	0.830	0.441	0.236
		0.271	0.634	0.323	0.121	0.224	0.752	0.487	0.262
		0.229	0.701	0.341	0.154	0.182	0.801	0.478	0.310

Auxiliary Information

Method/Apparatus/Procedure:

The method was not specified. Experiments were made at boiling temperatures of mixtures. The boiling temperatures of the two-liquid system were estimated by the compiler.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) source not specified.

Estimated Error:
temp. ± 1K (compiler).

Components:
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
H. Sugi and T. Katayama, J. Chem. Eng. Jpn. **10**, 400–2 (1977).

Variables:
T/K=298

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.0000	0.99949	0.0000	0.99989
		0.1701	0.7934	0.1290	0.8627
		0.2197	0.7222	0.1726	0.8137
		0.2606	0.6550	0.2127	0.7666
		0.2948	0.6067	0.2468	0.7284
		0.3166	0.5753	0.2697	0.7027
		0.3513	0.4932	0.3179	0.6399
		0.3645	0.4618	0.3379	0.6139
		0.3799	0.4305	0.3604	0.5857
		0.4149	0.3564	0.4172	0.5139
		0.4280	0.2842	0.4643	0.4421
		0.4282	0.2664	0.4748	0.4236
		0.4296	0.2423	0.4907	0.3969
		0.4293	0.2204	0.5048	0.3717
		0.4223	0.2008	0.5130	0.3498
		0.4117	0.1541	0.5397	0.2897
		0.3874	0.1044	0.5619	0.2171
		0.3609	0.0722	0.5689	0.1632
		0.3215	0.0496	0.5532	0.1224
		0.2815	0.0346	0.5251	0.0925
		0.2578	0.0280	0.5035	0.0784
		0.1827	0.0114	0.4146	0.0371

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase complier		water-rich phase complier	
25.0	298.2	0.3606	0.0732	0.1311	0.0029	0.5676	0.1652	0.3320	0.0105
		0.4200	0.1163	0.1253	0.0012	0.5787	0.2298	0.3222	0.0044
		0.4272	0.2229	0.1181	0.0007	0.5016	0.3753	0.3081	0.0026
		0.4170	0.3349	0.1155	0.0005	0.4292	0.4943	0.3030	0.0019
		0.3603	0.4766	0.1140	0.0003	0.3298	0.6255	0.3000	0.0011

Auxiliary Information

Method/Apparatus/Procedure:

The combination of a titration and analytical methods was used. The apparatus and experimental procedure were described in Ref. 1. For glc analysis of 1.6 m column filled with Poropak-Q was used. Solubility of water in hexane was determined by the Karl Fischer method.

Source and Purity of Materials:

Wako Chemicals Ind. Ltd., guaranteed reagent; dried with Molecular Sieve 3A, distilled; densities agreed within 0.0003 with literature values.
(2) Merck Uvasol, spectrograde; used as received; densities agreed within 0.0003 with literature values.
(3) de-ionized, twice distilled.

Estimated Error:
Not reported.

References:
[1] H. Sugi, T. Nitta, and T. Katayama, J. Chem. Eng. Jpn. **9**, 12 (1976).

Components:	**Evaluated by:**
(1)1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8] (2) Toluene (methylbenzene); C_7H_8; [108-88-3] (3) Water; H_2O; [7732-18-5]	A Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.02)

5.4. 1+Propanol + Water + Toluene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of 1-propanol between phases (distr.) for the system 1-propanol–toluene–water is given in Table 48.

TABLE 48. Summary of experimental data for the system 1-propanol–toluene–water

Author(s)	T/K	Type of data[a]	Ref.
Leikola, 1940	293	sat. (4)	1
Baker, 1955	298	sat. (16), eq. (11)	2
Nikurashina and Ilin, 1972	298	sat. (20), distr. (15)	3
Letcher and Siswana, 1992	298	sat. (15), eq. (8)	4

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 1-propanol–toluene–water forms a miscibility gap of type 1. Studies of the system were reported in four references and are discussed on the basis of original papers with the exception of data of Leikola,[1] which were taken from the handbook of Kafarov;[5] this data set was also taken into account during evaluation but is not reported as a compilation sheet because it does not contribute further to knowledge of the system. Only the toluene–water binary system forms a miscibility gap. The data for this binary system were compiled and critically evaluated in a previously published SDS volume.[6] The recommended values of mutual solubility of toluene–water system at 298 K are: $x_2'=0.9972$ and $x_2''=0.000\,104$.[6] The end points of saturation curve at 298.2 K,[4] were reported to be $x_2'=0.999$ and $x_2''=0.000$. These numerical results are limited by the accuracy of experimental measurements which were estimated by the authors to be 0.005 mole fraction; the data are within accuracy limit, but are not adequate to describe the regions of low concentrations of ethanol. Data reported by Ref. 4 show also a somewhat smaller (up to 0.03 mole fraction) concentration of water in the organic-rich phase (the region of 0.4–0.7 mole fraction of toluene) than data of other authors. A maximum value of 1-propanol concentration on the saturation curve at 298.2 K is reported to be $x_1=0.44$.[4] Concentration of toluene in the water-rich phase is very low, <0.002 mole fraction, so toluene was not reported in some experimental points in equilibrium, Ref. 4 (authors estimated composition of tie lines was within 0.01 mole fraction). All data describing the saturation curve are treated as tentative; they are consistent within each data set as well as between the references. Temperature of 298.2 K was selected to present the behavior of the system. The water-rich phase was not described by any equation and this phase is not presented in Table 48. All experimental saturation and equilibrium points of the hydrocarbon-rich phase at 298.2 K, were used to construct the equation:

$$x_1=0.788\,09+0.146\,55\ln(x_2)-0.542\,22x_2-0.245\,63x_2^2.$$

The least-squares method was used and the standard error of estimate was 0.0068. Calculated compositions of the hydrocarbon-rich part of the saturation curve are presented in Table 49 for the selected concentrations of toluene in the mixture. The results of calculations (solid line) are also presented graphically in Fig. 24 together with all experimental data reported at 298.2 K.

TABLE 49. Calculated composition along the saturation curve (hydrocarbon-rich phase) at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 104 Ref. 6	0.3439	0.5200
0.2038	0.0200	0.3334	0.5400
0.2943	0.0400	0.3224	0.5600
0.3424	0.0600	0.3111	0.5800
0.3730	0.0800	0.2995	0.6000
0.3940	0.1000	0.2874	0.6200
0.4088	0.1200	0.2751	0.6400
0.4192	0.1400	0.2623	0.6600
0.4265	0.1600	0.2493	0.6800
0.4312	0.1800	0.2359	0.7000
0.4340	0.2000	0.2222	0.7200
0.4350	0.2200	0.2082	0.7400
0.4347	0.2400	0.1939	0.7600
0.4331	0.2600	0.1793	0.7800
0.4305	0.2800	0.1644	0.8000
0.4269	0.3000	0.1492	0.8200
0.4224	0.3200	0.1338	0.8400
0.4172	0.3400	0.1180	0.8600
0.4113	0.3600	0.1020	0.8800
0.4048	0.3800	0.0857	0.9000
0.3976	0.4000	0.0691	0.9200
0.3899	0.4200	0.0523	0.9400
0.3816	0.4400	0.0352	0.9600
0.3729	0.4600	0.0179	0.9800
0.3637	0.4800	0.0091	0.9900
0.3540	0.5000	0.0000	0.9972 Ref. 6

Phases in equilibrium

The phases in equilibrium were measured at 298.2 K (Refs. 2 and 4). The tie lines cover the whole area of the miscibility gap and are consistent with one another. All experimental tie lines at 298.2 K together with the saturation curve are presented in Fig. 24. The plait point of the system at 298.2 K estimated by Letcher and Siswana[4] was $x_1=0.18$, $x_2=0.01$. Distribution of 1-propanol between hydrocarbon and water phases reported in Ref. 3 is in agreement with other equilibrium data. The characteristic point of the system, the same mass fraction concentration of 1-propanol in both phases (0.150),[3] after recalculation gives the values 0.21 and 0.048 mole fraction of 1-propanol in organic and water rich phases, respectively.

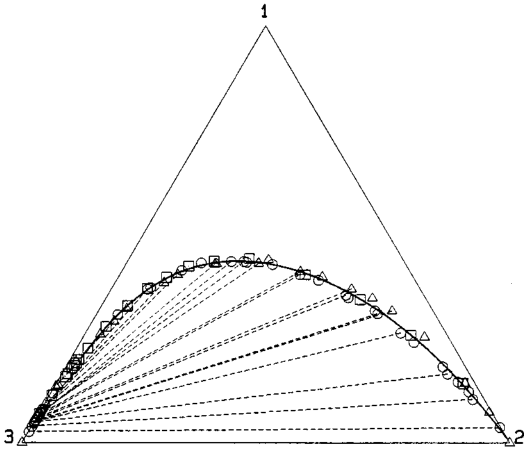

FIG. 24. Phase diagram of the system 1-propanol-toluene-water at 298.2 K. Solid line—calculated saturation curve, ○—experimental results of Ref. 2, □—experimental results of Ref. 3, △—experimental results of Ref. 4, dashed lines—experimental tie lines, Refs. 2 and 4.

References:

[1] E. Leikola, Suomen Kemistil. B **13**, 13 (1940).

[2] E. M. Baker, J. Phys. Chem. **59**, 1182 (1955)

[3] N. I. Nikurashina and K. K. Ilin, Zh. Obshch. Khim. **42**, 1657 (1972).

[4] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

[5] V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskva, 1963).

[6] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. M. Baker, J. Phys. Chem. **59**, 1182–3 (1955).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.122 21	0.854 22	0.084 93	0.910 16
		0.145 54	0.820 27	0.102 97	0.889 78
		0.181 77	0.771 06	0.131 90	0.857 84
		0.239 59	0.682 37	0.183 00	0.799 13
		0.315 27	0.564 64	0.259 06	0.711 36
		0.346 66	0.493 77	0.301 04	0.657 42
		0.389 02	0.412 18	0.360 01	0.584 84
		0.426 88	0.299 59	0.440 89	0.474 42
		0.432 29	0.244 45	0.478 20	0.414 60
		0.430 64	0.152 80	0.545 26	0.296 63
		0.371 67	0.078 38	0.565 96	0.182 99
		0.306 27	0.043 31	0.539 54	0.116 97
		0.191 57	0.013 44	0.425 25	0.045 73
		0.117 50	0.004 69	0.302 95	0.018 55
		0.081 18	0.001 42	0.226 53	0.006 09
		0.073 99	0.001 02	0.209 69	0.004 44

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.0370	0.9605	0.0262	0.0010	0.0245	0.9750	0.0820	0.0050
		0.1042	0.8716	0.0387	0.0010	0.0720	0.9230	0.1180	0.0045
		0.1645	0.7892	0.0467	0.0011	0.1185	0.8715	0.1400	0.0050
		0.2620	0.6443	0.0493	0.0009	0.2050	0.7730	0.1470	0.0040
		0.3082	0.5735	0.0524	0.0011	0.2520	0.7190	0.1550	0.0050
		0.3532	0.4861	0.0538	0.0006	0.3080	0.6500	0.1590	0.0025
		0.4027	0.3676	0.0607	0.0006	0.3890	0.5445	0.1770	0.0028
		0.4339	0.2382	0.0663	0.0008	0.4835	0.4070	0.1910	0.0035
		0.4341	0.2123	0.0671	0.0009	0.5015	0.3760	0.1930	0.0040
		0.4129	0.1214	0.0792	0.0013	0.5590	0.2520	0.2220	0.0055
		0.3672	0.0740	0.0801	0.0014	0.5665	0.1750	0.2240	0.0060

Auxiliary Information

Method/Apparatus/Procedure:

The titration and analytical methods were used. Weighed portions of 1-propanol and toluene in glass stoppered flasks were titrated with water from a calibrated burette. After each portion of water the mixture was shaken and the temperature of the solution was allowed to return to 25 °C before further additions of water. When the end-point was reached, the mixture was left in the bath for 30 min before specific gravity and refractive index were determined. The binary two liquid-phase mixtures of toluene and water were treated with 1-propanol and when equilibrium was reached the samples of each layer were removed and refractive indexes were determined. A large-scale graph of refractive index, constructed during the binodal curve determination, was used to find equilibrium concentrations.

Source and Purity of Materials:

(1) Eastman Kodak Co.; distilled over $CaCl_2$, middle fraction was used; $d(25\ °C,4\ °C)=0.799\,99\pm0.0002$, $n(25\ °C,D)=1.3854\pm0.0001$.
(2) source not specified; analytical reagent grade; dried over Na, distilled; $d(25\ °C,4\ °C)=0.859\,39\pm0.0002$, $n(25\ °C,D)=1.3325\pm0.0001$.
(3) distilled from alkaline potassium permanganate.

Estimated Error:

temp. ±0.1 °C.

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

N. I. Nikurashina and K. K. Ilin, Zh. Obshch. Khim. **42**, 1657–60 (1972). [Eng. transl. Russ. J. Gen. Chem. **42**, 1651–3 (1972)].

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.0697	0.0005	0.1996	0.0022
		0.1134	0.0039	0.2953	0.0155
		0.1579	0.0104	0.3731	0.0376
		0.1647	0.0111	0.3841	0.0398
		0.1783	0.0134	0.4042	0.0467
		0.1845	0.0144	0.4130	0.0495
		0.1908	0.0155	0.4216	0.0525
		0.1991	0.0170	0.4327	0.0567
		0.2256	0.0219	0.4654	0.0692
		0.2774	0.0337	0.5180	0.0964
		0.3283	0.0520	0.5529	0.1342
		0.3695	0.0727	0.5700	0.1720
		0.3960	0.0988	0.5666	0.2167
		0.4226	0.1309	0.5581	0.2651
		0.4346	0.1771	0.5284	0.3301
		0.4412	0.2452	0.4842	0.4126
		0.4028	0.3780	0.3843	0.5530
		0.3423	0.5209	0.2896	0.6757
		0.2563	0.6684	0.1966	0.7861
		0.1417	0.8326	0.0994	0.8952

Distribution of 1-propanol in 1-propanol–toluene–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_1'' water-rich phase
25.0	298.2	0.011	0.056
		0.038	0.101
		0.097	0.130
		0.150	0.150[a]
		0.218	0.155
		0.290	0.165
		0.358	0.174
		0.423	0.180
		0.480	0.188
		0.527	0.200
		0.561	0.211
		0.571	0.253
		0.537	0.291
		0.507	0.316
		0.467	0.351

[a] The same concentration of 1-propanol in both phases.

Auxiliary Information

Method/Apparatus/Procedure:

The isothermal titration method was used. Phase equilibrium was determined by the secants method.[1] Each secant represented a constant water-toluene mass ratio, the concentration of 1-propanol was variable. After 24 h separation, refractive indexes of both phases were measured. Equilibrium concentration of 1-propanol in both phases, in weight percent, was reported for 15 tie lines.

Source and Purity of Materials:

(1) source not specified, chemically pure grade: used as received; b.p.=97.4 °C, $n(20\ °\mathrm{C,D})=1.3858$.
(2) source not specified, pure for analysis grade: used as received; b.p.=110.6 °C, $n(20\ °\mathrm{C,D})=1.4967$.
(3) freshly distilled water; $n(20\ °\mathrm{C,D})=1.3332$.

Estimated Error:
temp. ±0.1 °C.

References:
[1] N. I. Nikurashina and R. V. Mertslin, *Metod Sechenii* (Izd. Saratovskii Universitet, Saratov, 1969).

Components:
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:
T/K=298

Compiled by:
A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.091	0.001	0.249	0.004
		0.138	0.005	0.343	0.019
		0.194	0.014	0.428	0.047
		0.259	0.031	0.499	0.092
		0.320	0.055	0.541	0.143
		0.403	0.118	0.554	0.249
		0.429	0.185	0.518	0.342
		0.438	0.286	0.457	0.457
		0.397	0.416	0.364	0.585
		0.346	0.544	0.285	0.688
		0.252	0.698	0.188	0.800
		0.143	0.836	0.100	0.896
		0.074	0.920	0.050	0.949
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1^{IH}	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/ °C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.315	0.600	0.049	0.000	0.250	0.730	0.147	0.000
		0.368	0.490	0.057	0.000	0.317	0.647	0.168	0.000
		0.410	0.365	0.064	0.000	0.395	0.540	0.186	0.000
		0.430	0.270	0.072	0.000	0.460	0.443	0.206	0.000
		0.428	0.182	0.080	0.000	0.519	0.339	0.225	0.000
		0.383	0.100	0.095	0.001	0.554	0.222	0.258	0.004
		0.290	0.044	0.135	0.002	0.521	0.121	0.340	0.008

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; $d=0.79979$, $n=1.3837$.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:
estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:
[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [17-23-8]
(2) 1-Heptene; C_7H_{14}; [592-76-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. M. Letcher, B. C. Bricknell, J. D. Sewry, and S. E. Radloff, J. Chem. Eng. Data **39**, 320–3 (1994).

Variables:
$T/\mathrm{K}=298$

Compiled by:
A. Skrzecz

5.5. 1-Propanol + Water + 1-Heptene

Experimental Data

Compositions along the saturation curve

$t/$ °C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	1.000	0.000	1.000
		0.080	0.901	0.051	0.945
		0.168	0.792	0.114	0.878
		0.287	0.622	0.216	0.764
		0.365	0.479	0.306	0.655
		0.416	0.343	0.397	0.534
		0.439	0.230	0.480	0.411
		0.433	0.154	0.536	0.311
		0.400	0.090	0.571	0.210
		0.316	0.040	0.550	0.114
		0.248	0.021	0.495	0.068
		0.186	0.010	0.420	0.037
		0.123	0.005	0.313	0.021
		0.026	0.001	0.081	0.005
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/$ °C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.365	0.060	0.150	0.010	0.509	0.178	0.300	0.043
		0.420	0.128	0.134	0.009	0.483	0.314	0.274	0.039
		0.420	0.326	0.112	0.008	0.346	0.572	0.237	0.036
		0.349	0.511	0.075	0.005	0.234	0.730	0.168	0.024
		0.132	0.838	0.026	0.002	0.068	0.926	0.063	0.010

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods have been described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) Aldrich; distilled; purity > 99.8 mole % by glc, $\rho=0.692\,65\ \mathrm{g\ cm^{-3}}$.
(3) not specified.

Estimated Error:
Not reported.

References:
[1] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:	**Evaluated by:**
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8] (2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.03)

5.6. 1-Propanol + Water + Heptane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-propanol–heptane–water is given in Table 50.

TABLE 50. Summary of experimental data for the system 1-propanol–heptane–water

Author(s)	T/K	Type of data[a]	Ref.
McCants *et al.*, 1953	311	sat. (15), eq. (4)	1
Vorobeva and Karapetyants, 1967	298	sat. (16), eq. (12)	2
Rabinovich and Pugachevich, 1974	293	eq. (5)	3
Timofeev *et al.*, 1975	348.7–349.5	eq. (5)	4
Letcher *et al.*, 1986	298	sat. (9), eq. (3)	5

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 1-propanol–heptane–water forms a large miscibility gap of type 1 covering the majority of the concentration triangle. The system was reported in the range 293–311 K and at the boiling point (vapor–liquid–liquid equilibria) at 101.3 kPa. Only the heptane–water binary system forms a miscibility gap. Data of this binary system were compiled and critically evaluated in a previously published SDS volume.[6] The recommended mutual solubilities of the binary system heptane–water at 298.2 K[6] are: $x_2''=4.3\cdot 10^{-7}$ and $x_3'=5.6\cdot 10^{-4}$. The solubility of water in heptane reported by Ref. 2 is 0.0055 mole fraction (0.001 weight fraction), which differs from the recommended value by a factor of 10. This is the result of the method used by Vorobeva and Karapetyants.[2] The data sets at 298.2 K,[2,5] are consistent with each other, with the exception of the region close to the plait point ($0.16<x_2<0.43$); Letcher *et al.*[5] present a slightly larger miscibility gap than Vorobeva and Karapetyants.[2] The temperature of 298.2 K, as a standard temperature in which various alcohol–hydrocarbon–water systems are presented, was chosen to present the behavior of this system. Saturation and equilibrium data of Refs. 2 and 5, were described by the equation:

$$x_1=a_1\cdot(-\ln z_1)^{a_2}\cdot z_1^{a_3},$$

where: $z_1=(x_2+0.5\cdot x_1-x_{20}'')/(x_{20}'-x_{20}'')$, x_1, x_2—mole fractions of component (1) and (2), respectively, x_{20}', x_{20}''—values of x_2 on the binodal curve which cuts the $x_1=0$ axis.

This equation has been proposed by Letcher *et al.*, Ref. 7, for the description of saturation curves of ternary alcohol–ether–water systems. It gives better results (the smallest standard deviation) for the investigated system than any other tested equation. The parameters obtained by the least-squares method for the whole range of miscibility gap (water-rich and hydrocarbon-rich branches were described together) are: $a_1=1.568\ 77$, $a_2=0.999\ 39$, $a_3=1.289\ 19$. The standard error of estimate was 0.0138. Points for selected concentrations of heptane on the saturation curve were calculated by the proposed equation. These are presented in Table 51 and Fig. 25 as calculated binodal curve (solid line). The maximum concentration of 1-propanol at this temperature is in the region of 0.470±0.025 ($x_1=0.486$, Ref. 5; $x_1=0.448$, calculated).

TABLE 51. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 000 43 Ref. 6	0.3551	0.5200
0.2539	0.0200	0.3439	0.5400
0.3137	0.0400	0.3322	0.5600
0.3522	0.0600	0.3202	0.5800
0.3797	0.0800	0.3078	0.6000
0.4001	0.1000	0.2950	0.6200
0.4155	0.1200	0.2818	0.6400
0.4270	0.1400	0.2684	0.6600
0.4354	0.1600	0.2546	0.6800
0.4414	0.1800	0.2405	0.7000
0.4452	0.2000	0.2261	0.7200
0.4472	0.2200	0.2115	0.7400
0.4477	0.2400	0.1965	0.7600
0.4468	0.2600	0.1813	0.7800
0.4447	0.2800	0.1659	0.8000
0.4414	0.3000	0.1502	0.8200
0.4372	0.3200	0.1343	0.8400
0.4321	0.3400	0.1182	0.8600
0.4261	0.3600	0.1018	0.8800
0.4194	0.3800	0.0853	0.9000
0.4120	0.4000	0.0685	0.9200
0.4039	0.4200	0.0515	0.9400
0.3952	0.4400	0.0344	0.9600
0.3859	0.4600	0.0170	0.9800
0.3762	0.4800	0.0000	0.999 44 Ref. 6
0.3659	0.5000		

Rabinovich and Pugachevich[3] measured the system at 293.2 K as two phases in equilibrium. This data set presents a much larger miscibility gap particularly in hydrocarbon-rich phase; for a similar alcohol concentration (e.g., 0.390 mole fraction) the heptane concentration at saturation point differs from the value at 298.2 K[2] by about 0.130 mole fraction. The compositions of the water-rich phase at 293.2 K are in agreement with other data sets. McCants *et al.*[1] report saturation and equilibrium data at 310.9 K. At this temperature, as was expected, data show a slightly smaller miscibility gap than those at 298.2 K. One point of the heptane-rich phase ($x_1=0.1922$ and $x_2=0.7009$) is an outlyer and presumably contains an experimental error. The paper of Timofeev, *et al.*[4] presents equilibrium data at normal boiling points. The compositions of the heptane-rich phase are consistent with the results at 298.2 K, but the reported concentrations of heptane in the water-rich phase seem abnormal high (0.04–0.06 mole fraction); (heptane concentrations at 298.2 K were measured to be about 0.01 mole fraction and the temperature dependence is not expected to result such large changes).

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 1-propanol–heptane–water were reported in all five references. The tie lines at 298.2 K (Refs. 2 and 5) are presented in Fig. 25. The distribution of 1-propanol between the phases changes slightly with the propanol concentration. This is observed in the data of Vorobeva and Karapetyants (Ref. 2) at 298.2 K. In the region $x_1<0.24$ the concentration of 1-propanol is slightly higher in the heptane-rich phase, while at higher alcohol concentrations, more 1-propanol is in the water-rich phase. Data of Letcher *et al.*[5] confirm this behavior for the low propanol region (all three tie lines are located in this region). Other tie lines, reported at various temperatures, show similar direction as at 298.2 K with the exception of the results of McCants *et al.*[1] These tie lines are in nearly the opposite direction (the direction of tie lines is consistent within this data set) than those presented in all other references. Plait points reported by Vorobeya and Karapetyants[2] at 298.2 K ($x_1=0.4255$ and $x_2=0.3090$) and Timofeev *et al.*[4] at 349.4 K ($x_1=0.43$ and $x_2=0.33$) are very close to one another. All experimental tie lines as well as experimental points on saturation curve, Refs. 2 and 5, at 298.2 K, are shown in Fig. 25.

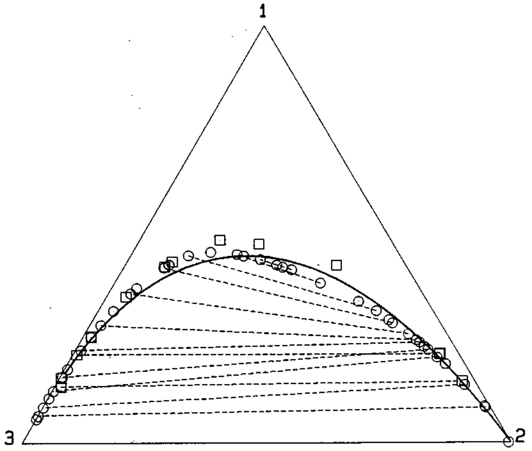

FIG. 25. Phase diagram of the system 1-propanol (1)—heptane (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 2, □—experimental data, Ref. 5, dashed lines—experimental tie lines, Refs. 2 and 5.

References:

[1] J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454 (1953).
[2] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144 (1969).
[3] I. I. Rabinovich and P. P. Pugachevich, Zh. Fiz. Khim. **48**, 2525 (1974).
[4] V. S. Timofeev, V. Yu. Aristovich, I. I. Sabylin, V. A. Koshel'kov, T. G. Pavlenko, and L. A. Serafimov, Izv. Vyssh, Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 1219 (1975).
[5] T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[6] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I. Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).
[7] T. M. Letcher, S. Ravindran, and S. E. Radloff, Fluid Phase Equilib. **69**, 251 (1991).

Components:	**Original Measurements:**
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8] (2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5] (3) Water; H_2O; [7732-18-5]	J. F. McCants, J. H. Jones, and W. H. Hopson, Ind. Eng. Chem. **45**, 454–6 (1953).

Variables:	**Compiled by:**
T/K=311	A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/ °F	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
100	310.9	0.0000	0.9945	0.000	0.999
		0.2283	0.7007	0.161	0.824
		0.3107	0.5645	0.241	0.730
		0.3598	0.4592	0.305	0.649
		0.4070	0.2983	0.410	0.501
		0.4312	0.2197	0.478	0.406
		0.4289	0.1314	0.550	0.281
		0.4072	0.0911	0.574	0.214
		0.3243	0.0413	0.556	0.118
		0.2689	0.0227	0.518	0.073
		0.1821	0.0092	0.414	0.035
		0.1193	0.0030	0.308	0.013
		0.0928	0.0015	0.253	0.007
		0.0448	0.0006	0.135	0.003
		0.0000	0.0002	0.000	0.001

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/ °F	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
100	310.9	0.1922	0.7009	0.1443	0.0024	0.138	0.839	0.357	0.010
		0.3240	0.5227	0.2526	0.0209	0.261	0.702	0.500	0.069a)
		0.3064	0.5574	0.2385	0.0183	0.240	0.728	0.485	0.062b)
		0.1912	0.7503	0.0883	0.0013	0.131	0.857	0.243	0.006c)

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to obtain binodal curve. The samples of homogeneous binary mixture were placed in a constant temperature bath and titrated the third component to the cloud point. Each sample was agitated in the constant temperature bath for several minutes between drops of the third component. The temperatures of these systems were raised slightly (1 °F) to obtain homogeneity and their refractive indexes were measured.
The analytical method was used for tie lines.
(a) A ternary mixture of known composition was shaken for several hours in constant temperature bath and after both phases were carefully separated and their refractive indexes were determined. The intersections of the tie lines with the binodal curve were determined by refractive index interpolations between points of known composition used to determine the curve.
(b) The slopes of the tie lines were checked by determining tie lines by the graphical application of the lever rule as described in Ref. 1.
(c) The two phases were analyzed chemically for one or two components.

Source and Purity of Materials:

(1) Du Pont, refined; used as received; $n(20\ ^\circ\mathrm{C,D})=1.3855$, $d(75\ ^\circ\mathrm{F},60\ ^\circ\mathrm{F})=0.800$.
(2) Philips, pure grade; used as received; $n(20\ ^\circ\mathrm{C,D})=1.3974$, $d(75\ ^\circ\mathrm{F},60\ ^\circ\mathrm{F})=0.680$.
(3) distilled; $n(20\ ^\circ\mathrm{C,D})=1.3330$.

Estimated Error:

refractive index ±0.0001; concentration ±0.001 mass % (estimated by compiler).

References:

[1] D. F. Othmer and P. E. Tobias, Ind. Eng. Chem. **34**, 690 (1942).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144-9 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 602–5 (1967)].

Variables:

$T/\mathrm{K}=298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/\ ^\circ\mathrm{C}$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9945	0.000	0.999
		0.0861	0.9032	0.054	0.944
		0.1861	0.7742	0.125	0.867
		0.2275	0.7105	0.159	0.828
		0.2919	0.6059	0.219	0.758
		0.3371	0.5212	0.270	0.696
		0.4200	0.3240	0.405	0.521
		0.4474	0.2305	0.482	0.414
		0.4566	0.1585	0.546	0.316
		0.4261	0.0889	0.592	0.206
		0.3697	0.0504	0.589	0.134
		0.3148	0.0307	0.560	0.091
		0.2522	0.0161	0.506	0.054
		0.1753	0.0059	0.407	0.023
		0.1070	0.0016	0.284	0.007
		0.0569	0.0006	0.167	0.003

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/\ ^\circ\mathrm{C}$	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.0831	0.9063	0.0644	0.0008	0.052	0.946	0.186	0.004
		0.1371	0.8372	0.0851	0.0009	0.089	0.906	0.236	0.004
		0.2022	0.7489	0.1239	0.0023	0.138	0.852	0.318	0.010
		0.2205	0.7218	0.1573	0.0045	0.153	0.835	0.378	0.018
		0.2382	0.6956	0.2205	0.0110	0.168	0.818	0.470	0.039
		0.2437	0.6859	0.2806	0.0221	0.173	0.812	0.533	0.070
		0.2581	0.6632	0.3566	0.0447	0.186	0.797	0.584	0.122
		0.2846	0.6168	0.4190	0.0821	0.212	0.766	0.594	0.194
		0.3141	0.5690	0.4484	0.1175	0.242	0.731	0.579	0.253
		0.3814	0.4205	0.4512	0.2150	0.334	0.614	0.496	0.394
		0.4141	0.3451	0.4386	0.2689	0.390	0.542	0.450	0.460
		0.4255	0.3090	0.4255	0.3090	0.417	0.505	0.417	0.505[a]

[a] Critical solubility point.

Auxiliary Information

Method/Apparatus/Procedure:

The methods were reported in Ref. 1. The titration method was used to describe solubility of the mixtures. The third component was added to the binary homogenous mixture until the cloudiness started to be observed. Density of the saturated mixtures was measured and put on the graphs. To obtain equilibrium ternary mixtures were stirred in thermostated vessel through several hours. After phase separation, density of each phase was measured and composition was determined from earlier prepared graphs. Concentration at critical point was found by the method described in Ref. 2. Water include in propanol was taken into account in all measurements.

Source and Purity of Materials:

(1) source not specified, chemical pure grade; distilled; water concentration was determined by the Karl Fischer method.
(2) source not specified; properties were the same as reported in Ref. 1.
(3) doubly distilled.

Estimated Error:

Not reported.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[2] E. N. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

I. I. Rabinovich and P. P. Pugachevich, Zh. Fiz. Khim. **48**, 2525-7 (1974). [Eng. transl. Russ. J. Phys. Chem. **48**, 1491–3 (1974)].

Variables:

T/K = 293

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
20.0	293.15	0.17	0.82	0.14	0.001	0.110	0.888	0.351	0.004
		0.23	0.73	0.27	0.02	0.158	0.834	0.523	0.065
		0.27	0.68	0.33	0.04	0.190	0.799	0.564	0.114
		0.33	0.62	0.40	0.07	0.239	0.750	0.592	0.173
		0.39	0.55	0.44	0.11	0.294	0.692	0.580	0.242

Comments and Additional Data

The authors described both branches of the solubility curve by the following equations obtained by the least-squares method.

$$x_1' = 0.6788 - 0.1927 x_3' - 49.0 x_3'^2$$

$$x_1'' = 0.0896 + 8.335 x_3'' - 3689.0 x_3''^2$$

Auxiliary Information

Method/Apparatus/Procedure:

Equilibrium data were obtained by the method reported in Ref. 1. The method uses experimental data of phases' density (measured in a three-capillary pycnometer) and the solubility curve (obtained by the method reported in Ref. 2). Solubility data were reported in the paper as the equations

Source and Purity of Materials:

(1) source not specified; chemically pure grade; used as received.
(2) source not specified; chemically pure grade; used as received.
(3) doubly distilled.

Estimated Error:

temp. ±0.1 °C.

References:

[1] P. P. Pugachevich and I. I. Rabinovich, Zh. Fiz. Khim. **45**, 2189 (1971).
[2] P. P. Pugachevich and I. I. Rabinovich, Zh. Fiz. Khim. **46**, 266 (1972).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. S. Timofeev, V. Yu. Aristovich, I. I. Sabylin, V. A. Koshel'kov, T. G. Pavlenko, and L. A. Serafimov, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. **18**, 1219–23 (1975).

Variables:

T/K=348.7–349.5

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C (compiler)	T/K	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
76.3	349.5	0.101	0.888	0.153	0.036	0.0637	0.9342	0.3354	0.1316
76.1	349.3	0.118	0.865	0.169	0.059	0.0754	0.9214	0.3388	0.1972
75.9	349.1	0.151	0.823	0.192	0.056	0.0986	0.8963	0.3759	0.1828
75.5	348.7	0.173	0.798	0.223	0.062	0.1144	0.8799	0.4124	0.1912
76.2	349.4	0.430	0.330	0.430	0.330	0.4087	0.5230	0.4087	0.5230[a]

[a] Critical solubility point.

Auxiliary Information

Method/Apparatus/Procedure:

The method is described in Ref. 1. Data are reported at the boiling point at 101.3 kPa together with liquid–liquid–vapor equilibrium data for the system.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] V. A. Koshelkov, T. G. Pavlenko, V. S. Timofeev, and L. A. Serafimov, Uch. Zap. Mosk. Inst. Tonkoi Khim. Tekhnol. **1**, 44 (1971).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:

T/K=298

Complied By:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.155	0.003	0.376	0.012
		0.253	0.016	0.507	0.053
		0.349	0.040	0.583	0.111
		0.422	0.082	0.597	0.193
		0.434	0.092	0.595	0.210
		0.486	0.163	0.563	0.315
		0.476	0.248	0.490	0.425
		0.425	0.432	0.358	0.606
		0.212	0.750	0.144	0.848

Compositions of coexisting phases

t/°C (compiler)	T/K	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (complier)		water-rich phase (compiler)	
		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
25	298.2	0.210	0.750	0.210	0.008	0.143	0.849	0.459	0.029
		0.146	0.828	0.135	0.013	0.095	0.900	0.328	0.053
		0.095	0.889	0.068	0.001	0.060	0.937	0.195	0.005

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) Merck, synthesis grade; dried with magnesium metal activated with iodine, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1] S. W. Briggs and E. W. Commings, Ind. Eng. Chem. **35**, 411 (1943).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053–60 (1989).

Variables:

$T/K=298$

Compiled by:

A. Skrzecz

5.7. 1-Propanol + Water + *p*-Xylene

Experimental Data

Compositions along the saturation curve

$t/°C$ (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.998	0.000	0.9997
		0.083	0.889	0.050	0.945
		0.157	0.798	0.099	0.892
		0.277	0.626	0.196	0.783
		0.358	0.474	0.287	0.672
		0.413	0.351	0.374	0.562
		0.441	0.251	0.451	0.454
		0.442	0.167	0.517	0.345
		0.408	0.099	0.558	0.239
		0.315	0.045	0.537	0.136
		0.260	0.028	0.497	0.095
		0.194	0.014	0.425	0.054
		0.138	0.006	0.341	0.026
		0.050	0.000	0.149	0.000
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (complier)		water-rich phase (complier)	
$t/°C$ (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
25.0	298.2	0.314	0.039	0.142	0.009	0.544	0.119	0.344	0.039
		0.426	0.123	0.078	0.004	0.547	0.279	0.217	0.020
		0.439	0.250	0.052	0.003	0.451	0.453	0.153	0.016
		0.385	0.418	0.038	0.002	0.326	0.624	0.115	0.011
		0.228	0.702	0.024	0.001	0.153	0.833	0.075	0.006

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. A binary mixture of known composition was titrated with the third component until cloudiness was observed. Tie line compositions were related to the coexistence curve; water was determined by the Karl Fischer titration. The methods were described in Ref. 1.

Source and Purity of Materials:

(1) source not specified; used as received.
(2) source not specified, recrystallized three times.
(3) not specified.

Estimated Error:

comp. <0.005 mole fraction (estimated authors' precision on binodal curve), <0.01 mole fraction (estimated authors' precision of tie lines).

References:

[1] T.M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

Components:	**Evaluated by:**
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8] (2)Octane (*n*-octane); C_8H_{18}; [111-65-9] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.05)

5.8. 1-Propanol + Water + Octane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-propanol–octane–water is given in Table 52.

TABLE 52. Summary of experimental data for the system 1-propanol–octane–water

Author(s)	T/K	Type of data[a]	Ref.
Vorobeva and Karapetyants, 1967	298	sat. (16), eq. (11)	1
Timofeev *et al.*, 1975	355–356	eq. (5)	2

[a] Number of experimental points in parentheses.

Saturation curve

The system 1-propanol–octane–water forms a miscibility gap of type 1. Only one binary pair of components, octane–water, is partially miscible. The data for this system were compiled and critically evaluated in a previously published SDS volume.[3] The recommended values of mutual solubility of octane–water system at 298.2 K are: $x_2''=1.1\cdot 10^{-7}$ and $x_2'=0.9994$. The solubility of water in octane reported in Ref. 1 as 0.001 mass fraction (equivalent to 0.006 mole fraction) is rejected because is inconsistent with recommended value.[3] Compositions along the saturation curve obtained by the titration method as well as compositions of phases in equilibrium are consistent at 298.2 K.[1] Data reported by Timofeev *et al.*[2] at very difficult experiments as vapor–liquid–liquid equilibria at 101.3 kPa and at boiling temperatures 354.7–355.7 K, present a larger miscibility gap than at 298 K, which indicates error in the experimental method. However they are consistent within the data set. On other hand, the data for the 1-propanol–octane–water system are consistent with the data for the 1-propanol–nonane–water system measured and reported by Vorobeva and Karapetyants in the same paper.[1]

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 1-propanol–octane–water were reported in both references. Composition of each phase was calculated from the density—composition curve of saturated mixtures prepared at the time of saturation curve measurements. Compositions of phases in equilibrium reported in Ref. 2 were measured only at boiling temperatures and detailed information about experimental procedures are not reported. Plait points were reported in both cases; at 298.2 K it is $x_1=0.449$ and $x_2=0.318$ and at 355.7 K—$x_1=0.540$ and $x_2=0.310$. All experimental data are treated as tentative. To present system behavior, the data at 298.2 K of Vorobeva and Karapetyant,[1] are presented in Fig. 26.

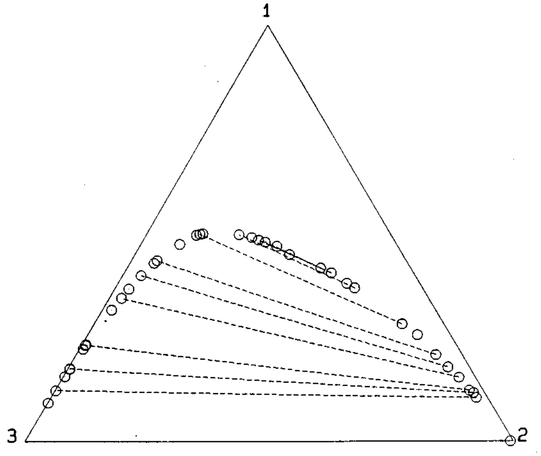

FIG. 26. Phase diagram of the system 1-propanol (1)—octane (2)—water (3) at 298.2 K. ○—experimental data, Ref. 1, dashed lines—experimental tie lines, Ref. 1.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144 (1967).

[2] V. S. Timofeev, V. Yu. Aristovich, I. I. Sabylin, V. A. Koshel'kov, T. G Pavlenko, and L. A. Serafimov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. 18, 1219 (1975).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Octane (*n*-octane); C_8H_{18}; [111-65-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144–9 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 602–5 (1967)].

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9937	0.000	0.999
		0.2561	0.6762	0.164	0.823
		0.3799	0.4705	0.288	0.678
		0.4697	0.2818	0.435	0.496
		0.4910	0.2200	0.493	0.420
		0.4996	0.1143	0.600	0.261
		0.4961	0.1030	0.611	0.241
		0.4746	0.0795	0.625	0.199
		0.4294	0.0493	0.632	0.138
		0.3673	0.0282	0.610	0.089
		0.3171	0.0180	0.576	0.062
		0.2337	0.0072	0.492	0.029
		0.2226	0.0069	0.477	0.028
		0.1749	0.0034	0.409	0.015
		0.1572	0.0024	0.380	0.011
		0.0933	0.0004	0.255	0.002

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (complier)		water-rich phase (complier)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.1044	0.8720	0.1232	0.0008	0.059	0.937	0.318	0.004
		0.1161	0.8605	0.1765	0.0032	0.066	0.930	0.412	0.014
		0.1221	0.8488	0.2319	0.0070	0.070	0.925	0.490	0.028
		0.1537	0.8121	0.3456	0.0238	0.090	0.904	0.596	0.078
		0.1785	0.7769	0.3996	0.0373	0.107	0.885	0.625	0.111
		0.2082	0.7376	0.4358	0.0522	0.128	0.862	0.633	0.144
		0.2823	0.6321	0.4987	0.1087	0.187	0.796	0.606	0.251
		0.3688	0.4921	0.4977	0.1906	0.274	0.695	0.522	0.380
		0.4050	0.4261	0.4847	0.2368	0.320	0.640	0.476	0.442
		0.4169	0.3985	0.4798	0.2529	0.339	0.616	0.461	0.462
		0.4495	0.3181	0.4495	0.3181	0.400	0.538	0.400	0.538[a]

[a] Critical solubility point.

Auxiliary Information

Method/Apparatus/Procedure:

The methods were reported in Ref. 1. The titration method was used to describe solubility of the mixtures. The third component was added to the binary homogenous mixture until the cloudiness started to be observed. Density of the saturated mixtures was measured and put on the graphs. To obtain equilibrium ternary mixtures were stirred in thermostated vessel through several hours. After phase separation, density of each phase was measured and composition was determined from earlier prepared graphs. Concentration at critical point was found by the method described in Ref. 2. Water include in propanol was taken into account in all measurements.

Source and Purity of Materials:

(1) source not specified, chemical pure grade; distilled; water concentration was determined by the Karl Fischer method.
(2) source not specified; properties were the same as reported in Ref. 1.
(3) doubly distilled.

Estimated Error: Not reported.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[2] E. N. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Octane (*n*-octane); C_8H_{18}; [111-65-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. S. Timofeev, V. Yu. Aristovich, I. I. Sabylin, V. A. Koshel'kov, T. G. Pavlenko, and L. A. Serafimov, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **18**, 1219–23 (1975).

Variables:

T/K=355–356

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
81.5	354.7	0.170	0.819	0.291	0.026	0.0983	0.8998	0.5338	0.0907
81.5	354.7	0.259	0.721	0.372	0.028	0.1584	0.8380	0.6148	0.0880
82.0	355.2	0.401	0.564	0.525	0.074	0.2703	0.7226	0.6680	0.1790
82.2	355.4	0.452	0.491	0.549	0.138	0.3223	0.6655	0.6065	0.2898
82.5	355.7	0.540	0.310	0.540	0.310	0.4599	0.5018	0.4599	0.5018[a]

[a] Critical solubility point.

Auxilliary Information

Method/Apparatus/Procedure:

The method is described in Ref. 1. Data are reported at the boiling point at 101.3 kPa together with liquid–liquid–vapor equilibrium data for the system.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] V. A. Koshelkov, T. G. Pavlenko, V. S. Timofeev, and L. A. Serafimov, Uch. Zap. Mosk. Inst. Tonkoi Khim. Tekhnol. **1**, 44 (1971).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12}; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

5.9. 1-Propanol + Water + Mesitylene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.070	0.000	0.201	0.000
		0.114	0.001	0.299	0.005
		0.165	0.006	0.388	0.028
		0.179	0.008	0.408	0.036
		0.220	0.016	0.457	0.067
		0.295	0.037	0.518	0.130
		0.379	0.081	0.539	0.230
		0.424	0.141	0.507	0.337
		0.435	0.218	0.446	0.447
		0.420	0.333	0.362	0.574
		0.381	0.444	0.288	0.672
		0.300	0.601	0.196	0.785
		0.175	0.789	0.099	0.895
		0.092	0.880	0.049	0.946
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.177	0.782	0.055	0.000	0.101	0.892	0.163	0.000
		0.289	0.615	0.070	0.000	0.187	0.795	0.201	0.000
		0.352	0.503	0.087	0.000	0.251	0.718	0.241	0.000
		0.422	0.320	0.098	0.001	0.370	0.562	0.265	0.005
		0.434	0.256	0.105	0.001	0.418	0.493	0.280	0.005
		0.425	0.159	0.117	0.002	0.490	0.366	0.304	0.010
		0.380	0.090	0.135	0.003	0.529	0.250	0.338	0.015

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; $d=0.79979$, $n=1.3837$.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Nonane (*n*-nonane); C_9H_{20} ; [111-84-2]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.04)

5.10. 1-Propanol + Water + Nonane

Critical Evaluation:

A survey of reported in the literature compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-propanol–nonane–water is given in Table 53.

TABLE 53. Summary of experimental data for the system 1-propanol–nonane–water

Author(s)	T/K	Type of data[a]	Ref.
Vorobeva and Karapetyants, 1967	298	sat. (12), eq. (13)	1
Koshelkov *et al.*, 1974	359–363	eq. (10)	2

[a] Number of expermental points in parentheses.

Saturation curve

The system 1-propanol–nonane–water forms a miscibility gap of type 1. Only one binary pair of components, nonane–water, is partially miscible. The data for this system were compiled and critically evaluated in a previously published SDS volumes, Ref. 3. The recommended values of mutual solubility of the nonane–water system at 298 K are: $x_2''=2.4\cdot 10^{-8}$ and $x_2'=0.999\ 44$. The solubility of water in nonane reported in Ref. 1 as 0.001 mass fraction (with the accuracy of ±0.001 of mass fraction equivalent to 0.007 mole fraction) is rejected. Data reported by Koshelkov *et al.*[2] represent vapor–liquid–liquid equilibria at boiling temperatures 358.7–363.2 K (pressure 101.3 kPa). Temperatures were estimated from the authors' graph. Compositions of the nonane-rich phase in the region $x_1>0.18$ seems to form a larger miscibility gap than at 298 K, which indicates an error in the experimental method of Ref. 2. Compositions at 298.2 K along the saturation curve obtained by titration method as well as compositions of phases in equilibrium are consistent in Ref. 1. These data are also consistent with the data of the 1-propanol–octane–water system reported by Vorobeva and Karapetyants in the same paper.[1]

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 1-propanol–nonane–water were reported in both references. Composition of each phase was calculated from density-composition curve of saturated mixtures prepared at the time of saturation curve measurements. Compositions of phases in equilibrium reported in Ref. 2 were measured only at boiling temperatures and detailed information about experimental procedures are not reported. A plait point reported at 298.2 K is $x_1=0.486$ and $x_2=0.318$ mole fraction. All experimental data are treated as tentative. To present the system behavior, the data at 298.2 K of Vorobeva and Karapetyant,[1] are presented in Fig. 27.

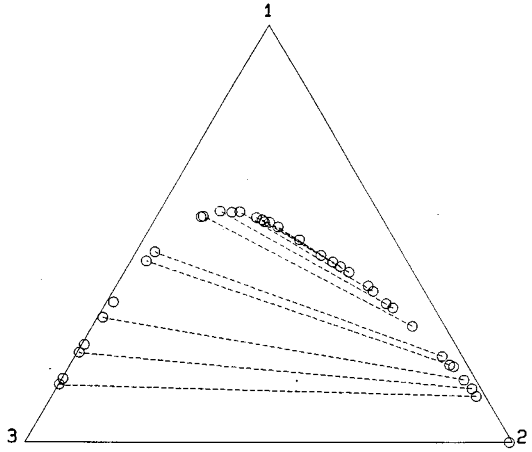

FIG. 27. Phase diagram of the system 1-propanol (1)—nonane (2)—water (3) at 298.2 K. ○—experimental data, Ref. 1, dashed lines—experimental tie lines, Ref. 1.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144 (1967).

[2] V. A. Koshelkov, T. G. Pavlenko, V. N. Titova, V. S. Timofeev, and L. A. Serafimov, Tr. Altai. Politekh. Inst. im. I. I. Polzunova **41**, 84 (1974).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

Components:	**Original Measurements:**
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8] (2) Nonane (*n*-nonane); C_9H_{20}; [111-84-2] (3) Water; H_2O; [7732-18-5]	A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144–9 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 602–5 (1967)].
Variables:	**Compiled by:**
T/K=298	A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9929	0.000	0.999
		0.1815	0.7873	0.097	0.898
		0.3324	0.5726	0.210	0.772
		0.3750	0.5145	0.249	0.729
		0.4487	0.3806	0.342	0.619
		0.5288	0.2254	0.488	0.444
		0.5516	0.1481	0.576	0.330
		0.5404	0.0906	0.640	0.229
		0.4567	0.0378	0.663	0.117
		0.3356	0.0134	0.600	0.051
		0.2336	0.0046	0.495	0.021
		0.1524	0.0011	0.373	0.006

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		Water-rich phase	
25	298.2	0.1105	0.8698	0.1386	0.0007	0.056	0.941	0.348	0.004
		0.1288	0.8516	0.2147	0.0036	0.066	0.931	0.470	0.017
		0.1496	0.8248	0.2989	0.0099	0.078	0.918	0.567	0.040
		0.1856	0.7773	0.4346	0.0313	0.100	0.894	0.657	0.101
		0.2059	0.7515	0.4562	0.0381	0.113	0.880	0.662	0.118
		0.2779	0.6543	0.5419	0.0942	0.164	0.824	0.636	0.236
		0.3222	0.5918	0.5543	0.1228	0.200	0.784	0.607	0.287
		0.3620	0.5310	0.5530	0.1638	0.237	0.742	0.560	0.354
		0.4081	0.4586	0.5390	0.2047	0.286	0.686	0.512	0.415
		0.4217	0.4343	0.5333	0.2192	0.303	0.666	0.496	0.435
		0.4326	0.4131	0.5275	0.2368	0.318	0.648	0.478	0.458
		0.4487	0.3806	0.5165	0.2596	0.342	0.619	0.454	0.487
		0.4858	0.3182	0.4858	0.3182	0.397	0.555	0.397	0.555[a]

[a] Critical solubility point.

Auxiliary Information

Method/Apparatus/Procedure:

The methods were reported in Ref. 1. The titration method was used to describe solubility of the mixtures. The third component was added to the binary homogenous mixture until the cloudiness started to be observed. Density of the saturated mixtures was measured and put on the graphs. To obtain equilibrium ternary mixtures were stirred in thermostated vessel through several hours. After phase separation, density of each phase was measured and composition was determined from earlier prepared graphs. Concentration at critical point was found by the method described in Ref. 2. Water include in propanol was taken into account in all measurements.

Source and Purity of Materials:

(1) source not specified, chemical pure grade; distilled; water concentration was determined by the Karl Fischer method.
(2) source not specified; properties were the same as reported in Ref. 1.
(3) doubly distilled.

Estimated Error:

Not reported.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[2] E. N. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Nonane (*n*-nonane); C_9H_{20}; [111-84-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. A. Koshelkov, T. G. Pavlenko, V. N. Titova, V. S. Timofeev, and L. A. Serafimov, Tr. Altai. Politekh. Inst. im. I. I. Polzunova **41**, 84–92 (1974).

Variables:

T/K=359–363

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		Water-rich phase (compiler)	
90.0	363.2	0.040	0.951	0.101	0.009	0.019	0.979	0.261	0.050
87.0	360.2	0.091	0.897	0.171	0.018	0.045	0.953	0.378	0.085
86.0	359.2	0.131	0.851	0.243	0.021	0.067	0.930	0.478	0.088
85.5	358.7	0.182	0.797	0.321	0.038	0.096	0.900	0.540	0.136
86.0	359.2	0.435	0.505	0.488	0.052	0.284	0.704	0.662	0.151
88.0	361.2	0.475	0.450	0.543	0.102	0.326	0.659	0.626	0.251

Auxiliary Information

Method/Apparatus/Procedure:

The method was not specified. Experiments were made at boiling temperatures of mixtures. Temperatures were read and estimated by the compiler from the authors' graphs.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) source not specified.

Estimated Error:

temp. ±0.5 K (compiler).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Decane (*n*-decane); $C_{10}H_{22}$; [124-18-5]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.01)

5.11. 1-Propanol + Water + Decane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-propanol–decane–water is given in Table 54.

TABLE 54. Summary of experimental data for the system 1-propanol–decane–water

Author(s)	T/K	Type of data[a]	Ref.
Dubovskaya and Karapetyants, 1968	293	sat. (17), eq. (4)	1
Mahers and Dawe, 1986	293	sat. (78), eq. (12)	2

[a] Number of experimental points in parentheses.

Saturation curve

Compositions along the saturation curve of the 1-propanol–decane–water system were obtained at 293.2 K by titration method, Refs. 1 and 2. All experimental solubility data at 293.2 K are presented in Fig. 1. Only one binary pair of components, decane–water, is partially miscible. Experimental values of mutual solubilities in this binary system were compiled and critically evaluated in a previously published SDS Volume, Ref. 3. At 293 K the tentative value for solubility of decane in water was reported to be $x_2''=2.5\cdot 10^{-9}$ while for solubility of water in decane reasonable data were not accessible; they are expected by the evaluator to be about $x_3'=6\cdot 10^{-4}$ mole fraction. Mutual solubilities of decane and water were not reported in the papers evaluated in Ref. 3. Compositions of four points in the water-rich phase at the lowest 1-propanol concentration were reported to be decane free,[2] which suggests that 1-propanol is only partially soluble in water. These numerical results are the consequence of the limited sensitivity of experimental measurements (reading the equilibrium phase composition from previously obtained curves of refractive index and density along the saturation curve). The concentration of the decane-rich phase (Ref. 2) in the range of $x_2>0.83$ appears to contain errors since it is inconsistent with the expected concentration of the binary mixture. The other experimental points of both types are consistent with one another and were fitted to the equation:

$$x_1=1.009\,02+0.133\,81\ln(x_2)-1.031\,32x_2-0.010\,20x_2^2.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0153. (The parameters describe experimental data which are in the region of 0.01–0.92 mole fraction of decane.) Points on the saturation curve calculated in the range of experimental data by the proposed equation are presented in Table 55 and in Fig. 28.

TABLE 55. Calculated composition along the saturation curve at 293.2 K

x_1	x_2	x_1	x_2
0.0000	$2.5\cdot 10^{-9}$ Ref. 3	0.4329	0.4600
0.3825	0.0100	0.4181	0.4800
0.4649	0.0200	0.4032	0.5000
0.5371	0.0400	0.3880	0.5200
0.5707	0.0600	0.3726	0.5400
0.5886	0.0800	0.3571	0.5600
0.5979	0.1000	0.3414	0.5800
0.6017	0.1200	0.3255	0.6000
0.6017	0.1400	0.3096	0.6200
0.5990	0.1600	0.2934	0.6400
0.5942	0.1800	0.2772	0.6600
0.5878	0.2000	0.2608	0.6800
0.5800	0.2200	0.2444	0.7000
0.5711	0.2400	0.2278	0.7200
0.5613	0.2600	0.2111	0.7400
0.5507	0.2800	0.1944	0.7600
0.5394	0.3000	0.1775	0.7800
0.5276	0.3200	0.1606	0.8000
0.5152	0.3400	0.1436	0.8200
0.5024	0.3600	0.1266	0.8400
0.4891	0.3800	0.1094	0.8600
0.4755	0.4000	0.0922	0.8800
0.4616	0.4200	0.0750	0.9000
0.4474	0.4400	0.0577	0.9200

Phase in equilibrium

Compositions of coexisting phases in equilibrium of the ternary system 1-propanol–decane–water were reported in two references. Similar experimental procedures were used in both references; when the equilibrium was reached then the phases were separated and the densities[1,2] and refractive indexes[2] of each phase were measured. The tie lines in each reference cover the whole area of the miscibility gap, but they are inconsistent with one another; the directions of the tie lines are quite different although the compositions of phases in equilibrium are located on the saturation curve. On the basis of tie lines consistency in a series 1-propanol–alkane–water systems,[4] the equilibrium data of Mahers and Dawe[2] appear to be more reasonable because they are similar to other systems. The equilibrium data of Dubovskaya and Karapetyants[1] are rejected.

The plait point estimated by Mahers and Dawe, Ref. 2, is $x_1=0.529$, $x_2=0.299$.

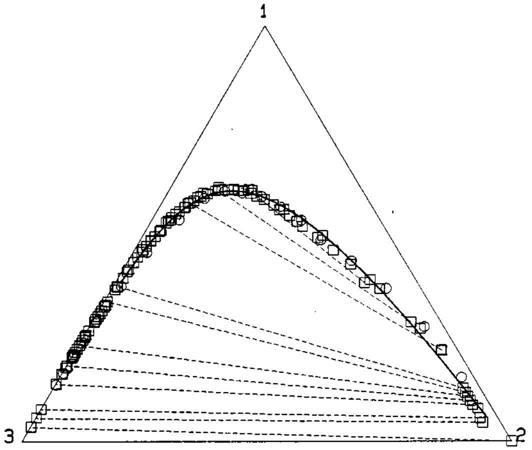

FIG. 28. Phase diagram of the system 1-propanol(1)—decane (2)—water (3) at 293.2 K. Solid line—calculated saturated curve, ○—experimental results of Ref. 1, □—experimental results of Ref. 2, dashed lines—experimental tie lines, Ref. 2.

References:

[1]A. S. Dubovskaya and M. Kh. Karapetyants, Tr. Inst.-Mosk., Khim.-Tekhnol. Inst. im. D. I. Mendeleeva **58**, 92 (1968).

[2]E. G. Mahers and R. A. Dawe, J. Chem. Eng. Data **31**, 28 (1986)

[3]D. G. Shaw, ed., *Solubility Data Series*, Vol. 38, Hydrocarbons with Water and Seawater, Part II; Hydrocarbons C_8 to C_{36} (Pergamon, New York, 1989).

[4]A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1144 (1967).

Components:	**Original Measurements:**
(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8] (2) Decane (*n*-decane); $C_{10}H_{22}$; [124-18-5] (3) Water; H_2O; [7732-18-5]	A. S. Dubovskaya and M. Kh. Karapetyants, Tr. Inst.-Mosk. Khim.-Tekhnol. Inst. im. D. I. Mendeleeva **58**, 92–7 (1968).
Variables: T/K=293	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
20.0	293.2	0.1537	0.8210	0.0730	0.9234
		0.2753	0.6846	0.1443	0.8494
		0.3671	0.5618	0.2136	0.7740
		0.4342	0.4577	0.2801	0.6990
		0.4846	0.3702	0.3450	0.6240
		0.5321	0.3063	0.4075	0.5554
		0.5645	0.2478	0.4675	0.4859
		0.5884	0.1978	0.5250	0.4178
		0.5974	0.1526	0.5780	0.3495
		0.6018	0.1154	0.6270	0.2847
		0.5846	0.0819	0.6655	0.2207
		0.5327	0.0552	0.6770	0.1660
		0.4548	0.0278	0.6730	0.0975
		0.3735	0.0159	0.6286	0.0634
		0.2886	0.0079	0.5570	0.0360
		0.1648	0.0022	0.3927	0.0123
		0.1369	0.0009	0.3444	0.0052

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20.0	293.2	0.2461	0.7087	0.1998	0.0030	0.1270	0.8660	0.4480	0.0160
		0.2721	0.6895	0.3304	0.0112	0.1420	0.8520	0.5960	0.0480
		0.3574	0.5731	0.5049	0.0426	0.2060	0.7820	0.6810	0.1360
		0.5758	0.2403	0.5758	0.2403	0.4800	0.4740	0.4800	0.4740[a]

[a]Critical point extrapolated by the authors, by Alekseev's method, Ref. 1.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine the solubility curve. Binary hydrocarbon–alcohol mixtures were titrated with water until turbidity was observed, as described in Ref. 1. The relationship of density versus composition of saturated mixture was used later to calculate equilibrium. The method was tested on the ethanol–heptane–water system and the results were in agreement with literature data. The analytical method was used to determine liquid–liquid equilibria. A binary mixture of known composition was placed in a special thermostated vessel and the third component was added to obtain a two-phase mixture. This mixture was agitated for 3–4 h to ensure equilibrium. The mixture was allowed to stand 1–2 h to became clear and then both phases were taken for density measurements. On the basis the previously constructed relationship of density versus composition of the saturated mixture, the composition of the mixture in equilibrium was calculated.

Source and Purity of Materials:

(1) source not specified; $d(20\ °C,20\ °C)=0.805$, $n(20\ °C,D)=1.3858$.
(2) source not specified; $d(20\ °C,20\ °C)=0.730$, $n(20\ °C,D)=1.4119$.
(3) double distilled.

Estimated Error:

temp. ±0.1 K; conc. ±0.0001.

References:

[1] W. D. Bancroft, Phys. Rev. **3**, 21 (1896).

Components:

(1) 1-Propanol (*n*-propanol, propyl alcohol, *n*-propyl alcohol); C_3H_8O; [71-23-8]
(2) Decane (*n*-decane); $C_{10}H_{22}$; [124-18-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. G. Mahers and R. A. Dawe, J. Chem. Eng. Data **31**, 28–31 (1986).

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
20.00	293.15	0.1629	0.0004	0.3930	0.0020
		0.1782	0.0004	0.4190	0.0020
		0.1821	0.0005	0.4250	0.0030
		0.2012	0.0007	0.4550	0.0040
		0.2045	0.0008	0.4600	0.0040
		0.2067	0.0009	0.4630	0.0050
		0.2097	0.0011	0.4670	0.0060
		0.2154	0.0010	0.4760	0.0050
		0.2222	0.0014	0.4850	0.0070
		0.2310	0.0016	0.4970	0.0080
		0.2378	0.0018	0.5060	0.0090
		0.2441	0.0020	0.5140	0.0100
		0.2516	0.0020	0.5240	0.0100
		0.2528	0.0018	0.5260	0.0090
		0.2566	0.0022	0.5300	0.0110
		0.2667	0.0027	0.5420	0.0130
		0.2882	0.0037	0.5660	0.0170
		0.2942	0.0032	0.5740	0.0150
		0.3008	0.0044	0.5790	0.0200
		0.3079	0.0049	0.5860	0.0220
		0.3148	0.0052	0.5910	0.0230
		0.3246	0.0055	0.6020	0.0240
		0.3379	0.0067	0.6140	0.0290
		0.1650	0.0072	0.6400	0.0300
		0.3711	0.0080	0.6440	0.0230
		0.3932	0.0095	0.6610	0.0380
		0.4086	0.0101	0.6730	0.0400
		0.4116	0.0109	0.6760	0.0420
		0.4309	0.0125	0.6870	0.0470
		0.4410	0.0146	0.6920	0.0540
		0.4569	0.0169	0.6980	0.0610
		0.4619	0.0164	0.7030	0.0590
		0.4700	0.0192	0.7030	0.0680
		0.4823	0.0225	0.7050	0.0780
		0.4842	0.0213	0.7090	0.0740
		0.4931	0.0253	0.7070	0.0860
		0.5059	0.0283	0.7100	0.0940
		0.5085	0.0297	0.7090	0.0980
		0.5264	0.0333	0.7140	0.1070
		0.5304	0.0341	0.7150	0.1090
		0.5324	0.0374	0.7100	0.1180

0.5380	0.0372	0.7140	0.1170
0.5474	0.0430	0.7090	0.1320
0.5517	0.0452	0.7090	0.1370
0.5611	0.0506	0.7050	0.1500
0.5641	0.0526	0.7020	0.1550
0.5724	0.0538	0.7050	0.1570
0.5782	0.0627	0.6930	0.1780
0.5868	0.0658	0.6920	0.1840
0.5890	0.0720	0.6840	0.1980
0.5973	0.0726	0.6880	0.1980
0.5951	0.0824	0.6710	0.2200
0.6020	0.0950	0.6560	0.2450
0.6113	0.0973	0.6580	0.2480
0.6054	0.1075	0.6400	0.2690
0.6043	0.1202	0.6220	0.2930
0.6064	0.1312	0.6090	0.3120
0.6030	0.1426	0.5910	0.3320
0.6022	0.1521	0.5810	0.3480
0.6026	0.1541	0.5790	0.3510
0.5967	0.1710	0.5570	0.3780
0.6029	0.1702	0.5620	0.3750
0.5899	0.1865	0.5370	0.4020
0.5817	0.2064	0.5110	0.4310
0.5691	0.2309	0.4840	0.4650
0.5572	0.2496	0.4620	0.4900
0.5582	0.2580	0.4560	0.4990
0.5428	0.2774	0.4310	0.5240
0.5170	0.3162	0.3930	0.5690
0.4906	0.3610	0.3530	0.6150
0.4956	0.3681	0.3520	0.6190
0.4601	0.4079	0.3140	0.6590
0.4262	0.4601	0.2750	0.7030
0.3880	0.5187	0.2360	0.7470
0.3669	0.5485	0.2170	0.7680
0.2707	0.6788	0.1410	0.8490
0.2180	0.7486	0.1090	0.8860
0.0792	0.8915	0.0360	0.9600

Compositions of coexisting phases

$t/°C$	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
20.00	293.15	0.0000	1.0000	0.0357	0.0000	0.0000	1.0000	0.1100	0.0000
		0.0446	0.9182	0.0578	0.0000	0.0200	0.9750	0.1700	0.0000
		0.0554	0.9077	0.0780	0.0000	0.0250	0.9700	0.2200	0.0000
		0.0869	0.8768	0.1390	0.0000	0.0400	0.9550	0.3500	0.0000
		0.0972	0.8668	0.1825	0.0009	0.0450	0.9500	0.4250	0.0050
		0.1073	0.8569	0.2331	0.0016	0.0500	0.9450	0.5000	0.0080
		0.1171	0.8471	0.3367	0.0058	0.0550	0.9400	0.6150	0.0250
		0.1272	0.8374	0.3734	0.0086	0.0600	0.9350	0.6450	0.0350
		0.2198	0.7469	0.5718	0.0571	0.1100	0.8850	0.7000	0.1650
		0.2865	0.6519	0.6049	0.1002	0.1550	0.8350	0.6500	0.2550
		0.3813	0.5105	0.6057	0.1638	0.2350	0.7450	0.5700	0.3650
		0.529	0.299	0.529	0.299	0.410	0.550	0.410	0.550[a]

[a] Estimated by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. The mass of each component added to the mixture was determined on an electronic balance. From the water-side of the system to 10 mL of water 1 drop of decane was added and then the mixture was titrated with 1-propanol until the mixture became homogenous. The decane-rich side of the system was determined similarly but starting with 10 mL of decane and adding water and 1-propanol. The refractive indexes and densities along the binodal curve were measured for selected compositions. The tie lines were determined by the analytical method. Two-phase mixtures were shaken well, then allowed to settle and samples of each phase were taken for analysis. Composition of equilibrium phases were derived from the refractive index and density curves.

Source and Purity of Materials:

(1) BDH, AnalaR grade; used as received; $n(20\ °C,D) = 1.385\ 32$, $\rho(20\ °C) = 803.9\ kg/m^3$.
(2) Koch-Light Ltd.; used as received; $n(20\ °C,D) = 1.412\ 13$, $\rho(20\ °C) = 710.0\ kg/m^3$.
(3) distilled.

Estimated Error:

temp. ±0.05 C.

6. 2-Propanol+Water

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Benzene; C_6H_6; [71-43-2]
(3)Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz. Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.04)

6.1. 2-Propanol + Water + Benzene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.), compositions of coexisting phases in equilibrium (eq.) and distribution of ethanol between phases (distr.) for the system 2-propanol–benzene–water is given in Table 56.

TABLE 56. Summary of experimental data for the system 2-propanol–benzene–water

Author(s)	T/K	Type of data[a]	Ref.
Perrakis, 1925	292	sat. (11)	1
Olsen and Washburn, 1935	298	sat. (16), distr. (15)	2
Leikola, 1940	293	sat. (4)	3
Udovenko and Mazanko, 1964	292–343	sat. (48), eq. (45)	4
Morachevskii and Legochkina, 1965	293–340	eq. (35)	5
Udovenko and Mazanko, 1967	303–323	eq. (23)	6
Nikurashina and Sinegubova, 1973	298	sat. (18), eq. (22)	7
Udovenko *et al.*, 1985	340	eq. (9)	8
Rajendran *et al.*, 1989	303	sat. (15), eq. (6)	9
Letcher *et al.*, 1990	298	sat. (13), eq. (5)	10

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 2-propanol–benzene–water forms a miscibility gap of type 1. Ten references describes this system over the temperature range 292–343 K. The data are evaluated on the basis of the original papers with the exception of data of Leikola,[3] which were taken from the handbook of Kafarov.[11] Experimental points reported in all ten papers are in general agreement. The data of Letcher *et al.*[10] were presented in graphical form only and therefore are not given as a compilation sheet. Only one binary system, benzene–water, is partially miscible. The data for this system were compiled and critically evaluated in a previously published SDS volume.[12] The recommended values of mutual solubility at 298.2 K[12] are: $x_2'=0.9970$ and $x_2''=0.000409$. Olsen and Washburn[2] and Rajendran *et al.*[9] reported mutual solubility for the binary system. These values at 298.2 K[2] and at 303.2 K[9] are: $x_2'=0.9970$, $x_2''=0.0003$ and $x_2'=0.9961$, $x_2''=0.0043$, respectively. The experimental results for the 2-propanol–benzene–water system of Perraksis[1] at 292 K are in agreement with other data sets, but the results for other alcohol–benzene–water systems reported in Ref. 1 differed very much from the recommended values. Therefore these data are not compiled. Data reported by Olsen and Washburn[2] at 298 K present a larger miscibility gap (by about 0.05 mole fraction) than any other data at a similar temperature. This was observed in the range $x_2=0.014–0.58$. The two points of lowest 2-propanol concentration in benzene-rich phase at 303 K, Rajendran *et al.*[9] are not located on the expected binodal curve. This is presumably the result of an experimental error. (Compositions are expected to contain of about 0.01 mole fraction less water.) Therefore the data of Refs. 2 and 9 are rejected. Udovenko and Mazanko[4] report five solubility–temperature curves of constant alcohol–benzene ratio and another four curves of constant alcohol–water ratio over the temperature range 292–343 K. These were used by the authors to construct solubility isotherms at 303, 318, and 333 K. Morachevskii and Legochkina[5] report equilibrium data in the temperature range 307–339 K. No significant compositional differences with temperature were observed on the binodal curve on the basis of these data sets. Saturation points at boiling temperatures as a function of pressure are also presented. The influence of composition on boiling temperature over two liquid phases at constant pressure is very weak; it changes no more than 0.5 K. All saturation data are treated as tentative. The temperature of 298.2 K was chosen to present the behavior of the system since several studies included this standard temperature. Saturation and equilibrium data of Nikurashina and Sinegubova[7] $(0.0004<x_2<0.9635)$, including water-rich and hydrocarbon-rich branches were described by the equation:

$$x_1=0.346\,81+0.042\,11\,\ln(x_2)+0.470\,10x_2-0.843\,39x_2^2.$$

The least-squares method was used and the standard error of estimate was 0.0125. The compositions on the saturation curve calculated by the proposed equation are presented in Table 57 for selected concentrations of benzene in the mixture. The results of calculations (solid line) are presented graphically in Fig. 29 together with all experimental data reported at 298.2 K.

TABLE 57. Calculated composition along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 409 Ref. 12	0.3472	0.4800
0.0564	0.0010	0.3418	0.5000
0.1575	0.0100	0.3357	0.5200
0.1911	0.0200	0.3288	0.5400
0.2287	0.0400	0.3212	0.5600
0.2535	0.0600	0.3128	0.5800
0.2727	0.0800	0.3037	0.6000
0.2884	0.1000	0.2939	0.6200
0.3018	0.1200	0.2834	0.6400
0.3133	0.1400	0.2722	0.6600
0.3233	0.1600	0.2603	0.6800
0.3319	0.1800	0.2476	0.7000
0.3393	0.2000	0.2342	0.7200
0.3456	0.2200	0.2202	0.7400
0.3523	0.2400	0.2054	0.7600
0.3510	0.2600	0.1899	0.7800
0.3587	0.2800	0.1737	0.8000
0.3612	0.3000	0.1568	0.8200
0.3629	0.3200	0.1393	0.8400
0.3637	0.3400	0.1210	0.8600
0.3637	0.3600	0.1020	0.8800
0.3629	0.3800	0.0810	0.9000
0.3613	0.4000	0.0620	0.9200
0.3589	0.4200	0.0409	0.9400
0.3558	0.4400	0.0191	0.9600
0.3519	0.4600	0.0000	0.9970 Ref. 12

No large differences in the maximum 2-propanol concentration were observed with temperature. The maximum 2-propanol concentration in benzene-rich phase of this ternary system at 298.2 K was measured to be $x_1=0.371$,[7] and $x_1=0.38$,[10] the value $x_1=0.41$ reported in Ref. 2 seems to be too large.

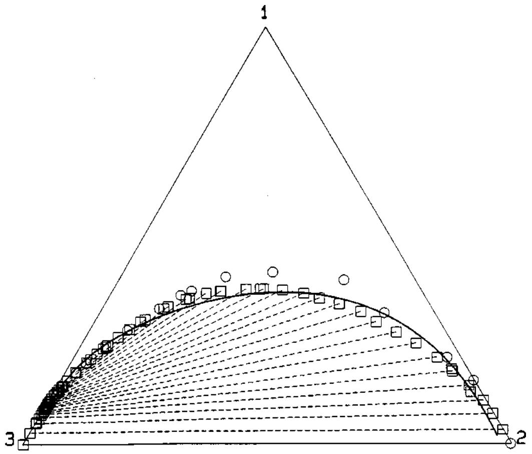

FIG. 29. Phase diagram of the system 2-propanol (1)—benzene (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 2, □—experimental data, Ref. 7, dashed lines—experimental tie lines, Ref. 2.

Phases in equilibrium

Compositions of coexisting phases in equilibrium of the ternary system 2-propanol–benzene–water were reported in seven references in the temperature range 293–340 K as 17 isotherms. The lines cover the full miscibility gap. Udovenko *et al.*[4,6,8] and Morachevskii and Legochikina[5] report the equilibrium data over the temperature range 303–340 K and 293–339 K, respectively. At various temperatures, tie lines systematically change direction slightly according to the final position of plait points. For constant water-phase composition, the benzene-rich phase in equilibrium contains less benzene at higher temperature. Reported data are consistent within each data set but several points are inconsistent between data sets, e.g., Ref. 4 at 303.2 K the composition of water-rich phase ($x_1=0.3251$ and $x_2=0.4885$) contains more alcohol than expected. Equilibrium data of Morachevskii and Legochkina at 293.2 K,[5] and Nikurashina and Sinegubova at 298.2 K,[7] are inconsistent with one another. All equilibrium data are treated as tentative. Plait point composition, reported in Refs. 4,7,10 and presented in Table 58 changes only slightly with temperature and contains less 2-propanol and more water at higher temperatures (concentration of benzene is nearly constant). This behavior is also confirmed by weak systematical changes of tie lines directions.[5] All experimental points at 298.2 K, both saturation and phases in equilibrium[2,7] are presented in Fig. 29.

TABLE 58. Experimental plait points for the system 2-propanol–benzene–water

T/K	x_1	x_2	Ref.
298.2	0.2299	0.0496	7
298.2	0.22	0.05	10
303.2	0.2248	0.0456	4
318.2	0.2188	0.0478	4
333.2	0.1970	0.0417	4

References:

[1] N. Perrakis, J. Chim. Phys. **22**, 280 (1925).

[2] A. L. Olsen and E. R. Washburn, J. Am. Chem. Soc. **57**, 303 (1935).

[3] E. Leikola, Suomen Kemistil B **13**, 13 (1940).

[4] V. V. Udovenko and T. F. Mazanko, Zh. Fiz. Khim. **38**, 2984 (1964).

[5] A. G. Morachevskii and L. A. Legochkina, Zh. Prikl. Khim. (Leningrad) **38**, 1789 (1965).

[6] V. V. Udovenko and T. F. Mazanko, Zh. Fiz. Khim. **41**, 395 (1967).

[7] N. I. Nikurashina and S. I. Sinegubova, Zh. Obshch. Khim. **43**, 2100 (1973).

[8] V. V. Udovenko, T. F. Mazanko, and V. Ya. Plyngeu, Izv. Akad. Nauk Mold. SSR, Ser. Biol. Khim. Nauk **3**, 52 (1985).

[9] M. Rajendran, S. Renganarayanan, and D. Srinivasan, Fluid Phase Equilib. **50**, 133 (1989).

[10] T. M. Letcher, J. Sewry, and S. Radloff, S. Afr. J. Chem. **43**, 56 (1990).

[11] V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskva, 1963).

[12] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:	**Original Measurements:**
(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0] (2) Benzene; C_6H_6; [71-43-2] (3) Water; H_2O; [7732-18-5]	A. L. Olsen and E. R. Washburn, J. Am. Chem. Soc. **57**, 303–5 (1935).
Variables: T/K=298	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
24.8	298.0	0.0000	0.9970	0.0000	0.9993
		0.1527	0.8448	0.1220	0.8774
		0.2081	0.7629	0.1722	0.8206
		0.3144	0.5816	0.2854	0.6863
		0.3930	0.4606	0.3795	0.5781
		0.4115	0.3066	0.4600	0.4455
		0.4005	0.2163	0.5028	0.3530
		0.3669	0.1627	0.5100	0.2940
		0.3570	0.1453	0.5136	0.2717
		0.3249	0.1172	0.5042	0.2363
		0.2737	0.0769	0.4816	0.1759
		0.1956	0.0314	0.4179	0.0871
		0.1729	0.0213	0.3911	0.0625
		0.1290	0.0067	0.3251	0.0221
		0.0922	0.0023	0.2516	0.0080
		0.0000	0.0003	0.0000	0.0015 data taken from Ref. 4.

Distribution of 2-propanol in 2-propanol–benzene–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_1'' water-rich phase
25.0	298.2	0.008	0.029
		0.015	0.058
		0.023	0.088
		0.033	0.113
		0.049	0.141
		0.089	0.179
		0.150	0.209
		0.198	0.228
		0.261	0.243
		0.301	0.256
		0.348	0.267
		0.389	0.279
		0.419	0.285
		0.443	0.297
		0.459	0.302

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. The method was described in Refs. 1,2,3. The mixtures were titrated at 24.8 °C in order that the slight excess necessary for the recognition of the end point, might be dissolved at 25.00 °C, the temperature at which the refractive indexes were determinated. The plot of refractive index against composition was used to find compositions of equilibrium phases. Phase equilibrium data were reported in incomplete form; only distribution of alcohol between water and benzene was reported. 20 mL of benzene and 20 mL of water were pipetted into glass stoppered bottles and varying amounts of alcohol were added to the mixture. The flasks were suspended in the thermostated water bath for a period of 24 h and occasionally shaking. After separation the layers were analyzed by means of refractometer and concentrations of alcohol were reported.

Source and Purity of Materials:

(1) source not specified; refluxed over lime, distilled; $d(25\ ^\circ\mathrm{C}) = 0.780\ 87$.
(2) source not specified; purified; $d(25\ ^\circ\mathrm{C}) = 0.873\ 44$.
(3) ''conductivity water''.

Estimated Error:

Not reported.

Reference:

[1] E. R. Washburn, V. Hnizda, and R. Vold, J. Am. Chem. Soc. **53**, 3237 (1931).
[2] R. Vold and E. R. Washburn, J. Am. Chem. Soc. **54**, 4217 (1932).
[3] E. R. Washburn and H. C. Spencer, J. Am. Chem. Soc. **56**, 361 (1934).
[4] *International Critical Tables*, Vol. 3 (McGraw-Hill, New York, 1929), p. 389.

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. V. Udovenko and T. F. Mazanko, Zh. Fiz. Khim. **38**, 2984–8 (1964) [Eng. transl. Russ. J. Phys. Chem. **38**, 1626–9 (1964)].

Variables:

T/K = 292–343

Compiled By:

A. Skrzecz

Experimental Data

		Compositions along the saturation curve			
	T/K	x_1	x_2	w_1	w_2
t/°C	(compiler)	(compiler)		(compiler)	
18.92	292.07	0.0559	0.0005	0.1647	0.0018
25.18	298.33	0.0559	0.0007	0.1646	0.0027
35.88	309.03	0.0559	0.0011	0.1643	0.0041
45.15	318.30	0.0559	0.0013	0.1642	0.0051
56.00	329.15	0.0558	0.0017	0.1639	0.0064
64.72	337.87	0.0558	0.0019	0.1638	0.0074
19.80	292.95	0.1111	0.0038	0.2912	0.0131
28.85	302.00	0.1109	0.0053	0.2898	0.0179
39.86	313.01	0.1108	0.0067	0.2884	0.0228
51.66	324.81	0.1106	0.0085	0.2867	0.0285
69.39	342.54	0.1103	0.0111	0.2841	0.0373
21.95	295.10	0.1960	0.0298	0.4199	0.0829
27.98	301.13	0.1956	0.0317	0.4176	0.0880
41.00	314.15	0.1949	0.0355	0.4131	0.0979
51.12	324.27	0.1946	0.0372	0.4111	0.1023
57.51	330.66	0.1941	0.0395	0.4084	0.1081
66.70	339.85	0.1937	0.0413	0.4063	0.1126
20.81	293.96	0.2809	0.0814	0.4861	0.1831
30.83	303.98	0.2802	0.0837	0.4834	0.1876
46.39	319.54	0.2794	0.0863	0.4803	0.1928
62.42	335.57	0.2784	0.0892	0.4768	0.1986
68.55	341.70	0.2778	0.0915	0.4742	0.2030
22.00	295.15	0.1807	0.7695	0.1511	0.8364
34.20	307.35	0.1797	0.7651	0.1509	0.8352
48.13	321.28	0.1789	0.7618	0.1507	0.8343
57.35	330.50	0.1780	0.7584	0.1505	0.8334
68.78	341.93	0.1775	0.7563	0.1504	0.8328
19.72	292.87	0.2880	0.5816	0.2659	0.6980
30.70	303.85	0.2867	0.5790	0.2656	0.6971
41.50	314.65	0.2856	0.5768	0.2653	0.6964
50.45	323.60	0.2843	0.5740	0.2650	0.6954
65.37	338.52	0.2818	0.5691	0.2643	0.6938
19.90	293.05	0.3675	0.3359	0.4115	0.4889
35.10	308.25	0.3637	0.3324	0.4101	0.4872
42.90	316.05	0.3622	0.3312	0.4095	0.4866
50.88	324.03	0.3596	0.3286	0.4085	0.4853
60.41	333.56	0.3566	0.3260	0.4073	0.4840
19.20	292.35	0.3592	0.1828	0.4893	0.3237
28.25	301.40	0.3562	0.1813	0.4876	0.3226
43.75	316.90	0.3511	0.1787	0.4847	0.3207
54.51	327.66	0.3469	0.1766	0.4823	0.3191
64.75	337.90	0.3421	0.1741	0.4795	0.3172
19.01	292.16	0.2591	0.0682	0.4716	0.1614
28.25	301.40	0.2530	0.0666	0.4655	0.1593
31.93	305.08	0.2488	0.0655	0.4612	0.1578
41.49	314.64	0.2424	0.0639	0.4545	0.1556
49.80	322.95	0.2357	0.0621	0.4474	0.1531
63.60	336.75	0.2288	0.0602	0.4398	0.1505

Compositions of coexisting phases

$t/°C$	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
30	303.2	0.0052	0.9905	0.0146	0.0002	0.004	0.995	0.047	0.001
		0.0219	0.9738	0.0292	0.0007	0.017	0.982	0.091	0.003
		0.0661	0.9254	0.0489	0.0010	0.052	0.946	0.146	0.004
		0.1302	0.8371	0.0650	0.0021	0.106	0.886	0.187	0.008
		0.2200	0.7101	0.0757	0.0027	0.189	0.793	0.213	0.010
		0.3042	0.5290	0.0897	0.0034	0.292	0.660	0.245	0.012
		0.3526	0.3764	0.1014	0.0049	0.382	0.530	0.270	0.017
		0.3640	0.3059	0.1130	0.0068	0.423	0.462	0.293	0.023
		0.3689	0.2544	0.1166	0.0072	0.454	0.407	0.300	0.024
		0.3619	0.2070	0.1237	0.0088	0.476	0.354	0.313	0.029
		0.3537	0.1788	0.1290	0.0092	0.487	0.320	0.323	0.030
		0.3512	0.1581	0.1416	0.0127	0.499	0.292	0.344	0.040
		0.3272	0.1228	0.1494	0.0152	0.502	0.245	0.356	0.047
		0.3029	0.0964	0.1650	0.0201	0.498	0.206	0.379	0.060
		0.2492	0.0628	0.2015	0.0344	0.464	0.152	0.424	0.094
		0.2248	0.0456	0.2248	0.0456	0.447	0.118	0.447	0.118[a]
45	318.2	0.0206	0.9709	0.0108	0.0007	0.016	0.982	0.035	0.003
		0.0534	0.9339	0.0221	0.0010	0.042	0.955	0.070	0.004
		0.1134	0.8537	0.0405	0.0013	0.092	0.900	0.123	0.005
		0.1860	0.7623	0.0545	0.0026	0.156	0.831	0.160	0.010
		0.2557	0.6330	0.0663	0.0030	0.230	0.740	0.190	0.011
		0.3103	0.5172	0.0738	0.0033	0.300	0.650	0.208	0.012
		0.3431	0.3999	0.0847	0.0045	0.365	0.553	0.233	0.016
		0.3601	0.3157	0.0953	0.0057	0.415	0.473	0.256	0.020
		0.3606	0.2367	0.1072	0.0080	0.457	0.390	0.280	0.027
		0.3543	0.1902	0.1177	0.0103	0.480	0.335	0.300	0.034
		0.3386	0.1542	0.1313	0.0147	0.490	0.290	0.323	0.047
		0.3100	0.1170	0.1459	0.0184	0.489	0.240	0.347	0.057
		0.2961	0.1022	0.1546	0.0215	0.486	0.218	0.360	0.065
		0.2447	0.0619	0.1898	0.0349	0.459	0.151	0.406	0.097
		0.2188	0.0478	0.2188	0.0478	0.437	0.124	0.437	0.124[a]
60	333.2	0.0231	0.9683	0.0083	0.0007	0.018	0.980	0.027	0.003
		0.0582	0.9249	0.0218	0.0015	0.046	0.950	0.069	0.006
		0.1222	0.8370	0.0374	0.0018	0.100	0.890	0.114	0.007
		0.1977	0.7247	0.0469	0.0023	0.170	0.810	0.140	0.009
		0.2445	0.6611	0.0545	0.0026	0.216	0.759	0.160	0.010
		0.3097	0.5089	0.0623	0.0029	0.302	0.645	0.180	0.011
		0.3544	0.3538	0.0731	0.0041	0.393	0.510	0.206	0.015
		0.3577	0.2720	0.0819	0.0053	0.435	0.430	0.226	0.019
		0.3502	0.1969	0.0996	0.0078	0.472	0.345	0.264	0.027
		0.3325	0.1530	0.1089	0.0101	0.485	0.290	0.282	0.034
		0.3132	0.1267	0.1252	0.0139	0.485	0.255	0.312	0.045
		0.2873	0.0976	0.1323	0.0160	0.480	0.212	0.324	0.051
		0.2520	0.0717	0.1522	0.0224	0.460	0.170	0.355	0.068
		0.1970	0.0417	0.1970	0.0417	0.411	0.113	0.411	0.113[a]

[a] Critical point of solubility.

Auxiliary Information

Method/Apparatus/Procedure:

Solubility was measured by the Alekseev's method.[1] Five solubility–temperature curves of constant alcohol–benzene ratio and another four curves of constant alcohol–water ratio were measured. These were used to construct solubility isotherms. Phase equilibrium was determined by comparison of density and refractive index on calibration curves obtained for saturation solutions. Critical points of solubility were obtained by the Alekseev's method.[2]

Source and Purity of Materials:

(1) source not specified; b.p.=81.4 °C at 750 Torr, $d(30\ °C, 4\ °C) = 0.7971$, $n(25\ °C, D) = 1.3749$.
(2) source not specified; purified; b.p.=79.0 °C at 752.5 Torr, $d(30\ °C, 4\ °C) = 0.8680$, $n(25\ °C, D) = 1.4980$; taken from Ref. 3.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] V. F. Alekseev, Gornyi Zh. **4**, 83 (1879).
[2] V. F. Alekseev, Gornyi Zh. **2**, 385 (1885).
[3] V. V. Udovenko and T. F. Mazanko, Zh. Fiz. Khim. **37**, 1151 (1963).

Components:
(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
A. G. Morachevskii and I. A. Legochkina, Zh. Prikl. Khim. (Leningrad) **38**, 1789–93 (1965). [Eng. transl. Russ. J. Appl. Chem. (Leningrad) **38**, 1751–4 (1965)].

Variables:
T/K = 293–340

Compiled by:
A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20.0	293.2	0.046	0.950	0.0561	0.0010	0.036	0.963	0.165	0.004
		0.204	0.747	0.0801	0.0019	0.172	0.816	0.224	0.007
		0.320	0.507	0.1065	0.0047	0.311	0.639	0.281	0.016
		0.366	0.333	0.1227	0.0063	0.412	0.487	0.313	0.021
		0.358	0.194	0.1444	0.0117	0.481	0.339	0.350	0.037
40.0	313.2	0.046	0.945	0.0419	0.0008	0.036	0.962	0.127	0.003
		0.220	0.710	0.0640	0.0016	0.189	0.793	0.185	0.006
		0.333	0.437	0.0815	0.0022	0.344	0.585	0.227	0.008
		0.360	0.290	0.0882	0.0028	0.428	0.448	0.242	0.010
		0.330	0.156	0.1050	0.0070	0.481	0.295	0.276	0.024
60.0	333.2	0.082	0.885	0.0306	0.0007	0.066	0.926	0.095	0.003
		0.230	0.675	0.0494	0.0015	0.203	0.772	0.147	0.006
		0.325	0.426	0.0633	0.0019	0.341	0.581	0.183	0.007
		0.346	0.318	0.0727	0.0024	0.403	0.480	0.206	0.009
		0.291	0.122	0.1092	0.0083	0.466	0.253	0.284	0.028

Compositions of coexisting phases

P/kPa	t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
			hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
26.7	34.32	307.47	0.075	0.913	0.0493	0.0010	0.059	0.938	0.147	0.004
	34.05	307.20	0.184	0.772	0.0636	0.0013	0.153	0.836	0.184	0.005
	34.26	307.41	0.269	0.610	0.0751	0.0019	0.245	0.722	0.212	0.007
	34.39	307.54	0.333	0.456	0.0868	0.0028	0.337	0.599	0.239	0.010
	34.52	307.67	0.362	0.305	0.0981	0.0046	0.422	0.462	0.263	0.016
53.3	50.18	323.33	0.085	0.890	0.0387	0.0017	0.068	0.926	0.118	0.005
	49.87	323.02	0.191	0.746	0.0520	0.0013	0.162	0.822	0.154	0.005
	49.97	323.12	0.274	0.586	0.0621	0.0016	0.254	0.707	0.180	0.006
	50.12	323.27	0.329	0.428	0.0728	0.0027	0.343	0.581	0.206	0.010
	50.36	323.51	0.352	0.288	0.0832	0.0039	0.422	0.449	0.230	0.014
80.0	60.27	333.42	0.090	0.873	0.0324	0.0012	0.073	0.918	0.100	0.005
	59.93	333.08	0.194	0.728	0.0449	0.0015	0.167	0.813	0.135	0.006
	59.97	333.12	0.274	0.570	0.0555	0.0018	0.258	0.698	0.163	0.007
	60.19	333.34	0.329	0.415	0.0658	0.0021	0.348	0.571	0.189	0.008
	60.47	333.62	0.346	0.275	0.0771	0.0030	0.423	0.438	0.216	0.011
101.3	66.57	339.72	0.095	0.864	0.0282	0.0015	0.077	0.913	0.088	0.006
	66.18	339.33	0.198	0.718	0.0402	0.0018	0.171	0.807	0.122	0.007
	66.19	339.34	0.276	0.562	0.0517	0.0018	0.262	0.692	0.153	0.007
	66.41	339.56	0.328	0.406	0.0618	0.0021	0.351	0.564	0.179	0.008
	66.71	339.86	0.345	0.272	0.0703	0.0027	0.424	0.435	0.200	0.010

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used in liquid–liquid equilibrium investigations. Samples of each phase were analyzed refractometrically as reported in Ref. 1. The solubility curve at 20 °C was also measured by the isothermal titration method; results were in agreement, but numerical data were not specified. The method and apparatus used in investigation of liquid–liquid vapor equilibrium were described in Ref. 2. Boiling temperatures of two-phase liquid mixtures were measured by Swietoslawski ebulliometer with a magnetic stirrer. Samples of each phase were analyzed refractometrically as reported in Ref. 1.

Source and Purity of Materials:

(1) source not specified; purified; $n(20\ °C,D) = 1.5010$, $d(20\ °C,4\ °C) = 0.8790$.
(2) source not specified; purified; $n(20\ °C,D) = 1.3771$, $d(20\ °C,4\ °C) = 0.7853$.
(3) not specified.

Estimated Error:

temp. ± 0.1 °C (accuracy of thermostating), ± 0.05 °C (accuracy of boiling temperature); comp. $< \pm 0.5$ mass %.

References

[1] A. G. Morachevskii and V. P. Belousov, Vest. Leningr. Univ., Ser. 4: Fiz. Khim. **4**, 118 (1958).
[2] N. A. Smirnova and A. G. Morachevskii, Vest. Leningr. Univ., Ser. 4: Fiz. Khim. **10**, 106 (1959).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Benzene: C_6H_6; [71-43-2]
(3) Water; H_2O [7732-18-5]

Original Measurements:

V. V. Udovenko and T. F. Mazanko, Zh. Fiz. Khim. **41**, 395–401 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 197–9 (1967)].

Variables:

T/K=303–333

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

t/°C (compiler)	T/K	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
30	303.2	0.0154	0.9760	0.0175	0.0005	0.012	0.986	0.056	0.002
		0.0370	0.9502	0.0394	0.0008	0.029	0.968	0.120	0.003
		0.0671	0.8956	0.0524	0.0018	0.054	0.937	0.155	0.007
		0.1435	0.8159	0.0683	0.0027	0.118	0.872	0.195	0.010
		0.1591	0.7850	0.0746	0.0033	0.133	0.853	0.210	0.012
		0.2605	0.6217	0.0859	0.0039	0.236	0.732	0.236	0.014
		0.3251	0.4885	0.1261	0.0061	0.320	0.625	0.320	0.020
45	318.2	0.0295	0.9619	0.0169	0.0005	0.023	0.975	0.054	0.002
		0.0938	0.8691	0.0369	0.0008	0.076	0.915	0.113	0.003
		0.1341	0.8253	0.0505	0.0018	0.110	0.880	0.150	0.007
		0.1911	0.7534	0.0564	0.0026	0.161	0.825	0.165	0.010
		0.2940	0.5634	0.0723	0.0038	0.275	0.685	0.204	0.014
		0.3544	0.3426	0.0889	0.0054	0.398	0.500	0.242	0.019
60	333.2	0.0231	0.9683	0.0098	0.0009	0.018	0.980	0.032	0.004
		0.0477	0.9229	0.0195	0.0015	0.038	0.955	0.062	0.006
		0.0975	0.8655	0.0338	0.0018	0.079	0.912	0.104	0.007
		0.1843	0.7378	0.0487	0.0021	0.158	0.822	0.145	0.008
		0.2075	0.7078	0.0513	0.0021	0.180	0.798	0.152	0.008
		0.2725	0.5779	0.0565	0.0032	0.255	0.703	0.165	0.012
		0.3007	0.5264	0.0621	0.0035	0.290	0.660	0.179	0.013
		0.3219	0.4503	0.0694	0.0041	0.330	0.600	0.197	0.015
		0.3577	0.2359	0.0864	0.0059	0.455	0.390	0.236	0.021
		0.3412	0.1796	0.1006	0.0079	0.475	0.325	0.266	0.027

Auxiliary Information

Method/Apparatus/Procedure:

The method was not reported. Liquid–liquid equilibrium data were presented together with vapor pressure and vapor composition over the two-phase liquid mixtures.

Source and Purity of Materials:

(1) source not specified; purified; b.p.=81.4 °C at 750 Torr, d(30 °C, 4 °C)=0.7971, n(25 °C,D)=1.3749.
(2) source not specified; purified; b.p.=79.0 °C at 752.5 Torr, d(30 °C,4 °C)=0.8680, n(25 °C,D)=1.4980.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

N. I. Nikurashina and S. I. Sinegubova, Zh. Obshch. Khim **43**, 2100-5 (1973). [Eng. transl. Russ. J. Gen. Chem. **43**, 2093-7 (1993)].

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
25	298.2	0.1246	0.8530	0.1005	0.8941
		0.1803	0.7857	0.1488	0.8428
		0.3354	0.4793	0.3308	0.6144
		0.3710	0.3018	0.4307	0.4554
		0.3664	0.2217	0.4709	0.3704
		0.3492	0.1672	0.4908	0.3055
		0.3246	0.1266	0.4966	0.2517
		0.2941	0.0941	0.4903	0.2039
		0.2759	0.0800	0.4816	0.1814
		0.2571	0.0660	0.4711	0.1571
		0.2373	0.0544	0.4560	0.1360
		0.2340	0.0520	0.4538	0.1311
		0.2299	0.0496	0.4504	0.1264
		0.2180	0.0426	0.4403	0.1119
		0.2051	0.0358	0.4280	0.0972
		0.1968	0.0314	0.4196	0.0870
		0.1377	0.0092	0.3397	0.0295
		0.0907	0.0019	0.2483	0.0068
		0.0540	0.0007	0.1596	0.0028

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.0344	0.9635	0.0277	0.0004	0.0267	0.9728	0.0867	0.0016
		0.0723	0.9243	0.0504	0.0007	0.0567	0.9425	0.1500	0.0028
		0.1041	0.8892	0.0626	0.0011	0.0825	0.9159	0.1816	0.0041
		0.1404	0.8414	0.0710	0.0013	0.1133	0.8823	0.2025	0.0047
		0.1747	0.7905	0.0762	0.0014	0.1441	0.8473	0.2150	0.0053
		0.2080	0.7429	0.0805	0.0018	0.1750	0.8126	0.2250	0.0065
		0.2419	0.6828	0.0838	0.0020	0.2100	0.7704	0.2325	0.0071
		0.2682	0.6297	0.0871	0.0021	0.2400	0.7326	0.2400	0.0076
		0.2928	0.5756	0.0915	0.0022	0.2710	0.6925	0.2500	0.0079
		0.3175	0.5326	0.0960	0.0023	0.3010	0.6564	0.2600	0.0081
		0.3359	0.4805	0.0988	0.0025	0.3308	0.6150	0.2660	0.0086
		0.3497	0.4321	0.1021	0.0026	0.3580	0.5750	0.2730	0.0091
		0.3608	0.3946	0.1058	0.0028	0.3810	0.5416	0.2810	0.0096
		0.3688	0.3480	0.1108	0.0035	0.4070	0.4993	0.2910	0.0118
		0.3716	0.3082	0.1180	0.0045	0.4280	0.4614	0.3050	0.0151
		0.3712	0.2726	0.1224	0.0055	0.4460	0.4257	0.3130	0.0183
		0.3668	0.2238	0.1266	0.0059	0.4700	0.3727	0.3210	0.0193
		0.3614	0.1955	0.1326	0.0069	0.4830	0.3395	0.3320	0.0223
		0.3470	0.1611	0.1416	0.0103	0.4930	0.2975	0.3460	0.0327
		0.3296	0.1326	0.1535	0.0134	0.4970	0.2599	0.3650	0.0413
		0.2989	0.1010	0.1739	0.0210	0.4900	0.2151	0.3930	0.0617
		0.2299	0.0496	0.2299	0.0496	0.4504	0.1264	0.4504	0.1264[a]

[a] Critical solubility point.

Auxiliary Information

Method/Apparatus/Procedure:

This isothermal titration method was used. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified, pure grade; used as received; b.p. = 82 °C, $n(25\ °C,D) = 1.3752$.

(2) source not specified; distilled at 80 °C; $n(25\ °C,D) = 1.5016$.

(3) doubly distilled.

Estimated Error:

Not reported.

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]

(2) Benzene; C_6H_6 ; [71-43-2]

(3) Water; H_2O; [7732-18-5]

Original Measurements:

V. V. Udovenko, T. F. Mazanko, and V. Ya. Plyngeu, Izv. Akad. Nauk Mold. SSR, Sef. Biol. Khim. Nauk **3**, 52–4 (1985).

Variables:

$T/K = 339.7-340.1$

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
66.90	340.05	0.0620	0.9280	0.0230	0.0030	0.0488	0.9489	0.0721	0.0122
66.70	339.85	0.1010	0.8840	0.0310	0.0030	0.0805	0.9159	0.0955	0.0120
66.50	339.65	0.1300	0.8420	0.0320	0.0050	0.1054	0.8877	0.0978	0.0199
66.52	339.67	0.2850	0.5150	0.0400	0.0070	0.2810	0.6599	0.1195	0.0272
66.55	339.70	0.3030	0.4650	0.0480	0.0080	0.3101	0.6187	0.1406	0.0305
66.60	339.75	0.3310	0.3740	0.0520	0.0090	0.3655	0.5368	0.1506	0.0339
66.65	339.80	0.3420	0.3280	0.0700	0.0100	0.3943	0.4916	0.1951	0.0362
66.70	339.85	0.3520	0.2700	0.0800	0.0100	0.4312	0.4299	0.2187	0.0355
66.80	339.95	0.3410	0.1810	0.1020	0.0130	0.4739	0.3270	0.2655	0.0440

Auxiliary Information

Method/Apparatus/Procedure:

The experimental method was not described. Liquid–liquid–vapor equilibrium data were reported at a pressure of 760 Torr. (Vapor composition over two-component liquid mixtures was also reported.) Initial binary water–benzene mixtures contained 25, 50, or 75 mass % water.

Source and Purity of Materials:

(1) source not specified; properties were described in Ref. 1.

(2) source not specified; properties were described in Ref. 1.

(3) not specified.

Estimated Error:

Not reported.

References:

[1] V. V. Udovenko, T. F. Mazanko, and V. Ya. Plyngeu, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **16,** 686 (1973).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. Rajendran, S. Renganarayanan, and D. Srinivasan, Fluid Phase Equilib. **50,** 133–64 (1989).

Variables:

T/K=303

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
30	303.2	0.0000	0.9961	0.0000	0.9991
		0.1237	0.8467	0.1003	0.8925
		0.2374	0.7108	0.2017	0.7851
		0.3263	0.5601	0.2998	0.6689
		0.3670	0.3926	0.3866	0.5375
		0.3704	0.2535	0.4558	0.4055
		0.3486	0.1491	0.5030	0.2797
		0.3036	0.0943	0.5004	0.2021
		0.2306	0.0549	0.4467	0.1383
		0.2024	0.0495	0.4123	0.1310
		0.1288	0.0138	0.3190	0.0443
		0.1114	0.0048	0.2912	0.0162
		0.0669	0.0037	0.1910	0.0138
		0.0304	0.0031	0.0939	0.0125
		0.0000	0.0043	0.0000	0.0184

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
30	303.2	0.0270	0.9411	0.01336	0.00520	0.0214	0.9710	0.0425	0.0215
		0.0599	0.9071	0.03144	0.00539	0.0480	0.9441	0.0961	0.0214
		0.2063	0.7347	0.06500	0.00529	0.1750	0.8100	0.1854	0.0196
		0.3057	0.5850	0.09267	0.00541	0.2782	0.6920	0.2504	0.0190
		0.3667	0.3894	0.11371	0.00503	0.3876	0.5351	0.2958	0.0170
		0.3617	0.1882	0.11247	0.00532	0.4880	0.3300	0.2930	0.0180

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities were determined at atmospheric pressure by a procedure described in Ref. 1. The concentration of 2-propanol was determined by glc using HP 5890-A microprocessor controlled unit and integrator HP 3390-A. A stainless steel column of 2 mm diameter packed with SE-30 (100% methyl silicone gum) and N_2 as carrier gas of 30 mL/min at 120 °C were used.

Source and Purity of Materials:

(1) Merck; reagent grade; purity>99.9% by glc.
(2) Merck; reagent grade; purity>99.9% by glc.
(3) double distilled.

Estimated Error:

temp. ±1 °C.

References:

[1] D. Rama Subramanian and D. Srinivasan, Chem. Eng. Commun. **19**, 335 (1983).

Components:	**Original Measurements:**
(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0] (2) Cyclohexene; C_6H_{10} ; [110-83-8] (3) Water; H_2O; [7732-18-5]	E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transue, J. Am. Chem. Soc. **62,** 1454–7 (1940).
Variables: T/K=288–308	**Compiled by:** A. Skrzecz

6.2. 2-Propanol + Water + Cyclohexene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
15.0	288.15	0.0273	0.9655	0.0202	0.9782
		0.1097	0.8694	0.0841	0.9111
		0.1954	0.7592	0.1570	0.8316
		0.2442	0.6841	0.2034	0.7787
		0.3018	0.5908	0.2644	0.7074
		0.3643	0.4385	0.3562	0.5860
		0.3935	0.2812	0.4495	0.4391
		0.3779	0.1700	0.5067	0.3116
		0.3272	0.1007	0.5142	0.2163
		0.2611	0.0441	0.4930	0.1138
		0.2332	0.0259	0.4752	0.0722
		0.1678	0.0065	0.3956	0.0209
		0.1449	0.0038	0.3576	0.0128
		0.1022	0.0009	0.2744	0.0034
		0.0820	0.0003	0.2294	0.0011
		0.0616	0.0003	0.1795	0.0011
		0.0313	0.0005	0.0972	0.0020
		0.0120	0.0002	0.0389	0.0008
25.0	298.15	0.0693	0.9105	0.0525	0.9429
		0.2125	0.7259	0.1737	0.8112
		0.3192	0.5461	0.2886	0.6749
		0.3781	0.3894	0.3858	0.5431
		0.3908	0.2899	0.4427	0.4489
		0.3685	0.1626	0.5039	0.3039
		0.3118	0.0833	0.5137	0.1876
		0.2621	0.0457	0.4927	0.1173
		0.2102	0.0204	0.4485	0.0594
		0.2017	0.0175	0.4387	0.0521
		0.1321	0.0037	0.3334	0.0129
		0.0714	0.0012	0.2034	0.0048
		0.0479	0.0009	0.1433	0.0035
		0.0224	0.0002	0.0710	0.0009
		0.0098	0.0001	0.0321	0.0006
35.0	308.15	0.0675	0.9075	0.0513	0.9430
		0.1789	0.7732	0.1431	0.8454
		0.3240	0.5392	0.2940	0.6688
		0.3893	0.3651	0.4047	0.5188
		0.3905	0.2494	0.4652	0.4062
		0.3747	0.1740	0.5010	0.3181
		0.3371	0.1135	0.5131	0.2362
		0.2721	0.0553	0.4953	0.1376
		0.2149	0.0255	0.4501	0.0731
		0.1242	0.0035	0.3180	0.0123
		0.0872	0.0012	0.2408	0.0046
		0.0480	0.0004	0.1439	0.0018
		0.0149	0.0001	0.0479	0.0006

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.15	0.0082	0.9873	0.0281	0.0002	0.006	0.993	0.088	0.001
		0.0750	0.9030	0.0691	0.0008	0.057	0.938	0.198	0.003
		0.2152	0.7236	0.1127	0.0019	0.176	0.809	0.296	0.007
		0.3228	0.5576	0.1406	0.0044	0.288	0.680	0.349	0.015
		0.3567	0.4624	0.1563	0.0070	0.342	0.606	0.375	0.023
		0.3863	0.3422	0.1768	0.0131	0.413	0.500	0.404	0.041
		0.3731	0.1707	0.2210	0.0242	0.502	0.314	0.460	0.069
		0.3274	0.0989	0.2487	0.0384	0.516	0.213	0.483	0.102

Distribution of 2-propanol in 2-propanol–cyclohexene–water system

t/°C	T/K (compiler)	w_1' hydrocarbon-rich phase	w_1'' water-rich phase
15.0	288.15	0.007	0.120
		0.035	0.205
		0.141	0.306
		0.232	0.361
		0.367	0.424
		0.473	0.473
		0.502	0.488
35.0	308.15	0.018	0.096
		0.049	0.172
		0.140	0.239
		0.247	0.299
		0.316	0.328
		0.365	0.345

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, as described in Ref. 1, was used. The titrant, from a weighed pipette, was added to the weighed binary mixture of known composition and the mixture was kept in a thermostated bath. To confirm that the end-point was reached the mixture was shaken automatically for at least 15 min and then reexamined. The plot of refractive index against composition was then used to find compositions of equilibrium phases. The refractive indexes were determinated at the temperature of 30.0 °C to eliminate an opalescence. Part of phase equilibrium data was reported in incomplete form; only distribution of alcohol between water and benzene was reported.

Source and Purity of Materials:

(1) Eastman Kodak Company, commercial grade; dried by refluxing over active lime, twice distilled; $d(25\ °C,4\ °C)=0.7809$, $n(25\ °C,D)=1.374\ 87$.
(2) Eastman Kodak Company, commercial grade; distilled in an atmosphere of purified N_2, collected in dried nitrogen-filled bottles; $d(25\ °C,4\ °C)=0.8056$, $n(25\ °C,D)=1.4434$.
(3) not specified.

Estimated Error:

temp. ±0.05 °C.

References:

[1]E. R. Washburn and A. E. Beguin, J. Am. Chem. Soc. **62**, 579 (1940).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]
(3) Water (hydrogen oxide); H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.04)

6.3. 2-Propanol + Water + Cyclohexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-propanol–cyclohexane–water is given in Table 59.

TABLE 59. Summary of experimental data for the system 2-propanol–cyclohexane–water

Author(s)	T/K	Type of data[a]	Ref.
Washburn *et al.*, 1942	298	sat. (13), eq. (8)	1
Verhoeye, 1968	298	sat. (27), eq. (8)	2
Nikurashina and Sinegubova, 1973	298	sat. (20), eq. (14)	3
Letcher *et al.*, 1991	298	sat. (14), eq. (6)	4
Plackov and Stern, 1992	298	sat. (21), eq. (7)	5

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 2-propanol–cyclohexane–water forms a miscibility gap of type 1. The system was studied five times at the same temperature, 298.2 K. Saturation data are consistent within and between each reference. The exceptions are two points for the cyclohexane-rich phase reported with the evident experimental errors in the paper of Verhoeye [2] ($x_1=0.213$ and $x_1=0.040$). Only one binary system, cyclohexane–water, forms a miscibility gap. The data for this binary system were compiled and critically evaluated in a previously published SDS volume, Ref. 6; the recommended values at 298.2 K are: $x_2''=1.2\cdot10^{-5}$ and $x_3'=3.7\cdot10^{-4}$. All experimental solubility and equilibrium data reported at 298.2 K were used for calculation of saturation curve. (Water-rich and hydrocarbon-rich branches were treated together.) These data were described by the equation:

$$x_1=0.475\,90+0.056\,28\ln(x_2)-0.113\,24x_2-0.58\,67x_2^2.$$

The parameters were calculated by the least-squares method and the standard error of estimate was 0.0156. Selected points on the saturation curve, calculated by the above equation are presented in Table 60 for selected concentrations of cyclohexane in the mixture and in Fig. 30 as calculated binodal curve (solid line).

TABLE 60. Calculated composition along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 012 Ref. 6	0.3438	0.5000
0.0873	0.0010	0.3361	0.5200
0.2178	0.0100	0.3278	0.5400
0.2578	0.0200	0.3189	0.5600
0.2983	0.0400	0.3095	0.5800
0.3222	0.0600	0.2996	0.6000
0.3390	0.0800	0.2891	0.6200
0.3517	0.1000	0.2780	0.6400
0.3615	0.1200	0.2665	0.6600
0.3694	0.1400	0.2544	0.6800
0.3756	0.1600	0.2417	0.7000
0.3804	0.1800	0.2286	0.7200
0.3840	0.2000	0.2149	0.7400
0.3866	0.2200	0.2007	0.7600
0.3883	0.2400	0.1860	0.7800
0.3891	0.2600	0.1708	0.8000
0.3890	0.2800	0.1550	0.8200
0.3882	0.3000	0.1388	0.8400
0.3867	0.3200	0.1220	0.8600
0.3845	0.3400	0.1047	0.8800
0.3816	0.3600	0.0870	0.9000
0.3780	0.3800	0.0687	0.9200
0.3738	0.4000	0.0499	0.9400
0.3690	0.4200	0.0306	0.9600
0.3636	0.4400	0.0108	0.9800
0.3576	0.4600	0.0007	0.9900
0.3510	0.4800	0.0000	0.999 63 Ref. 6

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 2-propanol–cyclohexane–water were reported in all references at 298.2 K and tie lines cover the full miscibility gap. The reported plait point, Ref. 3, was $x_1=0.3982$ and $x_2=0.2776$. In the area close to the plait point there are small differences in the direction of the tie lines. There is a nearly uniform distribution of alcohol between the phases, the concentration of 2-propanol in the equilibrium phases differs by no more than 0.03 mole fraction. In the water-rich phase, when $x_1<0.15$, the concentration of cyclohexane is very low, $x_2<0.002$. The reported equilibrium data sets are consistent with one another and within each data set. The exceptions are two points of the cyclohexane-rich phase reported with evident experimental errors in the paper of Verhoeye [2] (as discussed above in the description of saturation curve). The data for phases in equilibrium are considered tentative. All experimental tie lines as well as all experimental points, Refs. 1–5, at 298.2 K, are reported in Fig. 30.

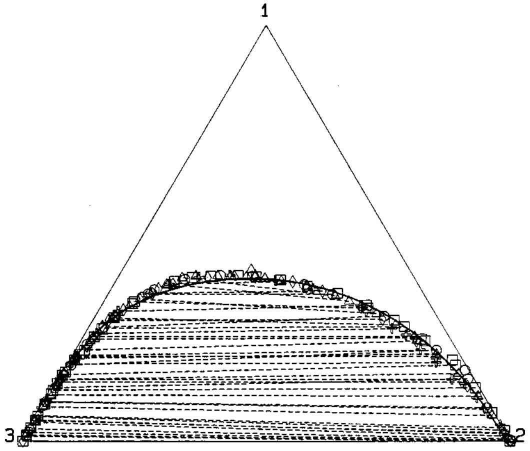

FIG. 30. Phase diagram of the system 2-propanol (1)—cyclohexane (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 1, □—experimental data, Ref. 2, △—experimental data, Ref. 3, ◇—experimental data, Ref. 4, ✚—experimental data, Ref. 5.

References:

[1] E. R. Washburn, C. E. Brockway, C. L. Graham, and P. Deming, J. Am. Chem. Soc. **64**, 1886 (1942).

[2] L. A. J. Verhoeye, J. Chem. Eng. Data **13**, 462 (1968).

[3] N. I. Nikurashina and S. I. Sinegubova, Zh. Obshch. Khim. **43**, 2100 (1973).

[4] T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118 (1991).

[5] D. Plackov and I. Stern, Fluid Phase Equilib. **71**, 189 (1992).

[6] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:	**Original Measurements:**
(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) Water; H_2O; [7732-18-5]	E. R. Washburn, C. E. Brockway, C. L. Graham, and P. Deming, J. Am. Chem. Soc. **64**, 1886–8 (1942).
Variables: T/K=298	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.0281	0.0003	0.0880	0.0014
		0.0862	0.0008	0.2388	0.0032
		0.1503	0.0032	0.3680	0.0108
		0.2320	0.0165	0.4829	0.0481
		0.2988	0.0414	0.5388	0.1046
		0.3449	0.0721	0.5557	0.1627
		0.3628	0.0882	0.5574	0.1897
		0.3875	0.1388	0.5353	0.2685
		0.3970	0.2069	0.4929	0.3597
		0.3952	0.2727	0.4508	0.4356
		0.3752	0.3894	0.3786	0.5502
		0.2992	0.5917	0.2578	0.7140
		0.1696	0.8216	0.1282	0.8698

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.0000	1.0000	0.0136	0.0004	0.000	1.000	0.044	0.002
		0.0028	0.9972	0.0224	0.0002	0.002	0.998	0.071	0.001
		0.0180	0.9773	0.0520	0.0012	0.013	0.986	0.154	0.005
		0.0801	0.9108	0.0950	0.0005	0.059	0.939	0.259	0.002
		0.1486	0.8382	0.1278	0.0025	0.112	0.885	0.326	0.009
		0.2179	0.7399	0.1814	0.0084	0.172	0.818	0.416	0.027
		0.2996	0.5920	0.2729	0.0299	0.258	0.714	0.521	0.080
		0.3521	0.4586	0.3529	0.0808	0.335	0.611	0.555	0.178

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, Refs. 1, 2, was used. Binary mixtures of known composition were titrated with the third component. The total weight of liquids employed was 13–15g . The refractive indexes of mixtures were used to construct the refractive index/composition curve, which was used further to find compositions of equilibrium phases.

Source and Purity of Materials:

(1) Eastman Kodak Company, best grade; dried with active lime, distilled; $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.7808$, $n(25\ °\mathrm{C,D})=1.3749$.
(2) Eastman Kodak Company; distilled, dried with Na, recrystallized several times; $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.7746$, $n(25\ °\mathrm{C,D})=1.4232$, f.p.$=6.1\ °\mathrm{C}$.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] R. Vold and E. R. Washburn, J. Am. Chem. Soc. **54**, 4217 (1932).
[2] E. R. Washburn and H. C. Spencer, J. Am. Chem. Soc. **56**, 361 (1934).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. A. J. Verhoeye, J. Chem. Eng. Data **13**, 462-7 (1968).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
25.0	298.2	0.0000	0.0002	0.0000	0.0010
		0.0156	0.0003	0.0500	0.0015
		0.0321	0.0007	0.0995	0.0030
		0.0502	0.0010	0.1495	0.0040
		0.0891	0.0014	0.2450	0.0055
		0.1134	0.0018	0.2975	0.0065
		0.1376	0.0026	0.3450	0.0090
		0.1660	0.0048	0.3940	0.0160
		0.1945	0.0092	0.4360	0.0290
		0.2082	0.0118	0.4540	0.0360
		0.2500	0.0219	0.5010	0.0615
		0.2956	0.0401	0.5365	0.1020
		0.3297	0.0601	0.5525	0.1410
		0.3821	0.1198	0.5465	0.2400
		0.3924	0.1507	0.5300	0.2850
		0.3952	0.1872	0.5050	0.3350
		0.3974	0.2430	0.4700	0.4025
		0.3939	0.2813	0.4450	0.4450
		0.3859	0.3353	0.4110	0.5000
		0.3715	0.3973	0.3725	0.5580
		0.3536	0.4690	0.3325	0.6175
		0.3263	0.5423	0.2900	0.6750
		0.2897	0.6176	0.2450	0.7315
		0.2443	0.6959	0.1975	0.7880
		0.1942	0.7842	0.1495	0.8455
		0.0684	0.9270	0.0500	0.9490
		0.0000	0.9977	0.0000	0.9995

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.026	0.974	0.060	0.001	0.019	0.981	0.175	0.004
		0.040	0.911	0.078	0.002	0.030	0.959	0.218	0.006
		0.127	0.864	0.121	0.002	0.095	0.903	0.312	0.009
		0.182	0.796	0.158	0.003	0.140	0.855	0.382	0.010
		0.213	0.787	0.184	0.007	0.162	0.838	0.422	0.021
		0.240	0.706	0.218	0.018	0.193	0.794	0.462	0.053
		0.274	0.646	0.269	0.028	0.228	0.752	0.518	0.075
		0.319	0.549	0.334	0.062	0.283	0.682	0.555	0.145

Auxiliary Information

Method/Apparatus/Procedure:

The binodal curve was determined by titration of heterogenous mixtures with a homogenous mixture until turbidity ceased. Two-liquid mixture was mixed for 1 h at constant temperature and after separation samples of each phase were analyzed. Liquid–liquid equilibrium data at boiling points (64.30–69.40 °C) at pressure 760 Torr were presented graphically in the paper.

Source and Purity of Materials:

(1) source not specified; distilled through a glass column (3 cm in diameter, 2 m high, packed in stainless wire) under reflux >10; chosen fractions were used; b.p. = 80.4 °C, $d(25\ °\mathrm{C},4\ °\mathrm{C}) = 0.7808$, $n(25\ °\mathrm{C},\mathrm{D}) = 1.3749$.
(2) source not specified; distilled through a glass column (3 cm in diameter, 2 m high, packed in stainless wire) under reflux >10; chosen fractions were used; b.p. = 80.7 °C, $d(25\ °\mathrm{C},4\ °\mathrm{C}) = 0.7738$, $n(25\ °\mathrm{C},\mathrm{D}) = 1.4238$.
(3) twice distilled.

Estimated Error:

temp. ±0.1 °C; comp. <0.0005 mole fraction (for the binodal curve).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

N. I. Nikurashina and S. I. Sinegubova, Zh. Obshch. Khim. **43**, 2100-5 (1973). [Eng. transl. Russ. J. Gen. Chem. **40**, 2093–7 (1973)].

Variables:

$T/\mathrm{K} = 298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°\mathrm{C}$	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.1388	0.0015	0.3481	0.0054
		0.1634	0.0033	0.3912	0.0109
		0.2412	0.0176	0.4942	0.0506
		0.2915	0.0360	0.5363	0.0927
		0.3243	0.0568	0.5502	0.1350
		0.3520	0.0809	0.5540	0.1784
		0.3743	0.1103	0.5478	0.2261
		0.3966	0.1568	0.5287	0.2928
		0.3961	0.2012	0.4960	0.3528
		0.3963	0.2285	0.4782	0.3861
		0.3954	0.2364	0.4725	0.3956
		0.4110	0.2629	0.4687	0.4198
		0.3938	0.2615	0.4561	0.4242
		0.3928	0.2801	0.4448	0.4442
		0.3982	0.2776	0.4504	0.4397
		0.3894	0.3015	0.4306	0.4669
		0.3836	0.3378	0.4080	0.5032
		0.3712	0.3976	0.3722	0.5583
		0.3217	0.5362	0.2885	0.6733
		0.2408	0.6880	0.1965	0.7861

Compositions of coexisting phases

		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
$t/°\mathrm{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
25	298.2	0.0022	0.9964	0.0161	0.0001	0.0016	0.9981	0.0516	0.0003
		0.0059	0.9918	0.0323	0.0002	0.0042	0.9953	0.1000	0.0007
		0.0116	0.9852	0.0460	0.0004	0.0083	0.9910	0.1383	0.0015
		0.0322	0.9641	0.0632	0.0005	0.0233	0.9759	0.1833	0.0020
		0.0615	0.9312	0.0831	0.0006	0.0450	0.9534	0.2316	0.0025
		0.1074	0.8792	0.1102	0.0009	0.0800	0.9170	0.2916	0.0035
		0.1612	0.8130	0.1481	0.0021	0.1233	0.8708	0.3650	0.0074
		0.2088	0.7444	0.1992	0.0077	0.1650	0.8239	0.4450	0.0240
		0.2506	0.6789	0.2503	0.0203	0.2050	0.7777	0.5033	0.0571
		0.2781	0.6259	0.2943	0.0387	0.2350	0.7407	0.5366	0.0988
		0.3053	0.5733	0.3408	0.0704	0.2667	0.7015	0.5533	0.1601
		0.3350	0.5018	0.3754	0.1072	0.3083	0.6467	0.5516	0.2205
		0.3471	0.4674	0.3913	0.1311	0.3283	0.6191	0.5450	0.2556
		0.3982	0.2776	0.3982	0.2776	0.4504	0.4397	0.4504	0.4397[a]

[a] Critical solubility point.

Auxiliary Information

Method/Apparatus/Procedure:

The isothermal titration method was used. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified, pure grade; used as received; b.p. = 82 °C, $n(25\ °\mathrm{C,D}) = 1.3752$.
(2) source not specified; distilled at 80.8 °C; $n(25\ °\mathrm{C,D}) = 1.4238$.
(3) doubly distilled.

Estimated Error:

Not reported.

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118–21 (1991).

Variables:

$T/\mathrm{K} = 298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°\mathrm{C}$	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.140	0.004	0.348	0.014
		0.198	0.011	0.439	0.034
		0.275	0.026	0.528	0.070
		0.315	0.049	0.549	0.119
		0.365	0.096	0.552	0.203
		0.392	0.183	0.505	0.330
		0.394	0.280	0.446	0.444
		0.370	0.396	0.372	0.558
		0.320	0.534	0.288	0.673
		0.240	0.688	0.196	0.786
		0.131	0.846	0.099	0.896
		0.068	0.923	0.050	0.948
		0.000	0.999	0.0000	0.9998

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
$t/°\mathrm{C}$	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.141	0.830	0.141	0.004	0.107	0.886	0.350	0.014
		0.203	0.746	0.202	0.012	0.161	0.827	0.445	0.037
		0.247	0.680	0.245	0.021	0.202	0.780	0.496	0.059
		0.292	0.592	0.290	0.032	0.253	0.717	0.539	0.083
		0.359	0.435	0.354	0.089	0.349	0.591	0.548	0.193
		0.382	0.362	0.376	0.120	0.396	0.525	0.541	0.242

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the titration method, as described in Ref. 1. The formation of a cloudy mixture was observed visually on shaking after addition of a known mass of the third component; syringes were precisely weighed. Tie line compositions were determined by the refractive index method, Ref. 2, and a complementary method using the Karl Fischer titration, Ref. 3. Measurements were made at pressure of 94.7 kPa.

Source and Purity of Materials:

(1) Merck; AR grade; refluxed with Mg and I_2, distilled; purity >99.9 mole % by glc.
(2) BDH; Gold label grade; used as received; purity >99.9 mole % by glc.
(3) not specified.

Estimated Error:

composition ±0.005 mole fraction (binodal curve), ±0.01 mole fraction (tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. Plackov and I. Stern, Fluid Phase Equilib. **71**, 189–209 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.0378	0.9601	0.0273	0.9722
		0.1031	0.8793	0.0770	0.9191
		0.1359	0.8384	0.1031	0.8910
		0.1982	0.7497	0.1568	0.8308
		0.2534	0.6608	0.2104	0.7683
		0.3105	0.5500	0.2766	0.6861
		0.3632	0.4141	0.3596	0.5742
		0.3841	0.3260	0.4141	0.4922
		0.3966	0.2270	0.4794	0.3842
		0.3909	0.1665	0.5165	0.3081
		0.3747	0.1147	0.5443	0.2333
		0.3547	0.0856	0.5522	0.1866
		0.3030	0.0442	0.5405	0.1104
		0.2258	0.0197	0.4708	0.0575
		0.1880	0.0081	0.4269	0.0258
		0.1624	0.0043	0.3883	0.0144
		0.1314	0.0026	0.3330	0.0092
		0.0981	0.0006	0.2658	0.0023
		0.0790	0.0004	0.2222	0.0016
		0.0508	0.0003	0.1513	0.0013
		0.0220	0.0002	0.0698	0.0009

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25	298.2	0.020	0.977	0.051	0.000	0.014	0.985	0.152	0.000
		0.077	0.908	0.096	0.002	0.057	0.940	0.260	0.008
		0.147	0.807	0.146	0.004	0.114	0.875	0.359	0.014
		0.188	0.755	0.184	0.007	0.149	0.838	0.422	0.022
		0.218	0.708	0.203	0.009	0.177	0.805	0.449	0.028
		0.269	0.624	0.257	0.024	0.229	0.744	0.508	0.066
		0.325	0.531	0.311	0.041	0.292	0.669	0.553	0.102

Auxiliary Information

Method/Apparatus/Procedure:

Binodal compositions were determined by titration with the corresponding, less-soluble component until the appearance of turbidity.[1] The analytical method was used for determination of tie-lines. This was based on refractive indexes and densities of the samples,[1] combined with the oxidation of the alcohol with an excess of potassium dichromate and determination of unreduced dichromate with $Na_2S_2O_3$. Alcohol in the organic layer was determined after extraction with water.

Source and Purity of Materials:

(1) Kemika (Zagreb); analytical grade; presumably used as received; $n=1.3475$, $\rho(25\ °C)=780.8\ kg/m^3$, b.p.$=81.1\ °C$.
(2) Merck Alkaloid; purity not specified; presumably used as received; $n=1.4232$, $\rho(25\ °C)=773.4\ kg/m^3$, b.p.$=80.1\ °C$.
(3) twice distilled in the presence of $KMnO_4$.

Estimated Error:

composition <0.0005 mass fraction, binodal, (relative); composition ±2%, tie line.

References:

[1] D. Plackov, and I. Stern, Fluid Phase Equilib. **57**, 327 (1990).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.05)

6.4. 2-Propanol + Water + Hexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-propanol–hexane–water is given in Table 61.

TABLE 61. Summary of experimental data for the system 2-propanol–hexane–water

Author(s)	T/K	Type of data[a]	Ref.
Vorobeva and Karapetyants, 1967	298	sat. (11), eq. (12)	1
Morozov *et al.*, 1978	331	eq. (6)	2

[a] Number of experimental points in parentheses.

Saturation curve

The system 2-propanol–hexane–water forms a miscibility gap of type 1. Compositions along the saturation curve was reported only in Ref. 1 at 298 K. Only one binary pair of components, hexane–water, is partially miscible. The data for this system were compiled and critically evaluated in a previously published SDS volume.[3] The recommended values of mutual solubility of hexane–water system at 298.2 K are: $x_2'=0.999\ 53$ and $x_2''=2.3\cdot 10^{-6}$. Two compositions in equilibrium at 331.2 K[2] were reported to be binary mixtures (concentration of the third component became equal 0.0). It seems that the analytical method used (glc) did not detect low concentrations of water and therefore these data are treated as inaccurate.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 2–propanol–hexane–water were reported in both references. There is no distribution of alcohol between the phases at 298.2 K[1] (concentration of 2-propanol expressed in mole fractions is practically constant). Composition of a plait point obtained graphically by the authors of Ref. 1 is equal to $x_1=0.416$ and $x_2=0.240$. Equilibrium data at 298.2 K are in agreement with data on the saturation curve and are also consistent with other ternary systems 2-propanol–hydrocarbon–water reported in Ref. 1. The larger miscibility gap and different direction of tie lines at 331.2 K than those at 298.2 K further show that the data of Ref. 2 are inaccurate. The data of Vorobeva and Karapetyants[1] at 298.2 K are treated as tentative and they are presented in Fig. 31.

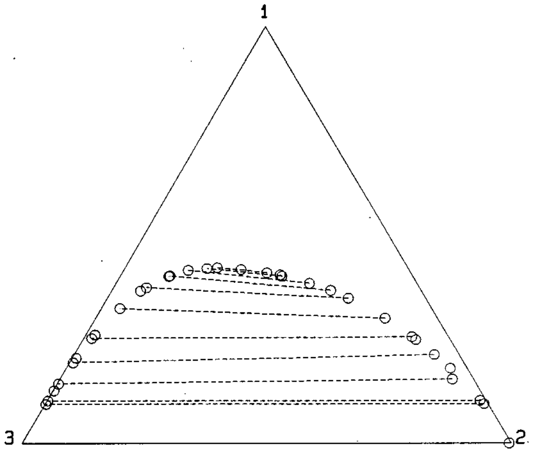

FIG. 31. Phase diagram of the system 2-propanol (1)—hexane (2)—water (3) at 298.2 K. ○—experimental data, Ref. 1, dashed lines—experimental tie lines, Ref. 1.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim, **41**, 1984 (1967).

[2] A. V. Morozov, A. G. Sarkisov, V. B. Turovskii, and V. I. Ilyaskin, Dep. Doc. VINITI **102–78**, 1 (1978).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:	**Original Measurements:**
(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0] (2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3] (3) Water; H_2O; [7732-18-5]	A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1984–9 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 1061–3 (1967)].
Variables: T/K=298	**Compiled by:** A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/ °C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9952	0.000	0.999
		0.1790	0.7858	0.136	0.856
		0.2480	0.6813	0.199	0.784
		0.3476	0.4941	0.315	0.642
		0.4030	0.3269	0.423	0.492
		0.4203	0.1888	0.520	0.335
		0.3994	0.0994	0.577	0.206
		0.3649	0.0585	0.587	0.135
		0.2601	0.0179	0.518	0.051
		0.2039	0.0076	0.452	0.024
		0.1263	0.0014	0.324	0.005

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/ °C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.094	0.897	0.0939	0.0010	0.068	0.930	0.256	0.004
		0.102	0.885	0.1020	0.0010	0.074	0.923	0.274	0.004
		0.153	0.803	0.1424	0.0025	0.116	0.874	0.354	0.009
		0.212	0.737	0.1930	0.0068	0.165	0.823	0.436	0.022
		0.255	0.670	0.2517	0.0155	0.206	0.776	0.510	0.045
		0.300	0.593	0.3235	0.0373	0.254	0.719	0.569	0.094
		0.348	0.494	0.3729	0.0666	0.315	0.642	0.586	0.150
		0.366	0.449	0.4003	0.1013	0.344	0.604	0.576	0.209
		0.383	0.397	0.4141	0.1320	0.376	0.559	0.560	0.256
		0.400	0.332	0.4185	0.1683	0.418	0.498	0.534	0.308
		0.408	0.297	0.4203	0.1888	0.442	0.462	0.520	0.335
		0.416	0.240	0.416	0.240	0.482	0.398	0.482	0.398[a]

[a] Critical point obtained graphically by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods were described in Ref. 1. Water impurities in alcohol were taken into account in the measurements. Critical point of liquid–liquid equilibrium was obtained graphically by the method reported in Ref. 2.

Source and Purity of Materials:

(1) source and method of preparation were reported in Ref. 1.
(2) source not specified; pure grade; distilled; water concentration was analyzed by the Karl Fischer method.
(3) doubly distilled.

Estimated Error:
Not specified.

References:
[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[2] E. F. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. V. Morozov, A. G. Sarkisov, V. B. Turovskii, and V. I. Ilyaskin, Dep. Doc. VINITI **102–78**, 1–9 (1978).

Variables:
$T/\mathrm{K}=331$

Compiled by:
A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/$ °C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
58	331.2	0.123	0.877	0.0425	0.0000	0.089	0.911	0.129	0.000
		0.171	0.829	0.1046	0.0004	0.126	0.874	0.280	0.0015
		0.289	0.601	0.1635	0.0035	0.244	0.728	0.391	0.012
		0.332	0.487	0.2880	0.0255	0.306	0.644	0.543	0.069
		0.399	0.341	0.3744	0.1113	0.413	0.506	0.544	0.232
		0.396	0.178	0.3957	0.1782	0.508	0.328	0.508	0.328

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The compositions of both phases were determined by glc.

Source and Purity of Materials:

(1) source not specified; dried, distilled, $n(20\ °\mathrm{C,D})=1.3771$, $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.7829$.
(2) source not specified; twice distilled, $n(20\ °\mathrm{C,D})=1.3748$, $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.6544$.
(3) doubly distilled.

Estimated Error:
comp. $<5\%$ relative, max. for water.

Components:
(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Evaluated by:
A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.03)

6.5. 2-Propanol + Water + Toluene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-propanol–toluene–water is given in Table 62.

TABLE 62. Summary of experimental data for the system 2-propanol–toluene–water

Author(s)	T/K	Type of data[a]	Ref.
Leikola, 1940	293	sat. (4)	1
Washburn and Beguin, 1940	298	sat. (24), eq. (13)	2
Stankova *et al.*, 1970	293, 349–352	sat. (52)	3
Borisova *et al.*, 1978	293, 349–354	eq. (17)	4
Letcher and Siswana, 1992	298	sat. (14), eq. (6)	5

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 2-propanol–toluene–water forms a miscibility gap of type 1. The system was measured at 293 K, 298 K, and at boiling temperatures at 101.3 kPa. Only toluene–water binary system forms a miscibility gap. The data of this binary system were compiled and critically evaluated in a previously published SDS volume.[6] The recommended values of mutual solubility of toluene–water system at 298 K are: $x_2'=0.9972$ and $x_2''=0.000\,104$.[6] This critical evaluation is based on the original papers with the exception of data of Leikola,[1] which were taken from the handbook of Kafarov;[7] this data set was also taken into account during evaluation but is not reported as a compilation sheet because it does not contribute further to knowledge of the system. At 293 K the experimental data of Borisova *et al.*[4] present a slightly larger miscibility gap than those of Stankova *et al.*[3] which are very close to the results at 298 K. The data for the saturation curve are consistent within each data set, as well as with one another. The miscibility gap decreases with increasing temperature. A maximum value of 2-propanol concentration on saturation curve observed at 298 K is equal to $x_1=0.39\pm0.01$ (differences between data sets, Refs. 2,5 are about 0.02 mole fraction). The saturation curve was described by the equation proposed by Hlavaty[8] and used also with success by Letcher *et al.*[9] for the description of saturation curves of ternary systems containing alcohols

$$x_1=a_1\cdot z_1\cdot\ln(z_1)+a_2\cdot z_2\ln(z_2)+a_3\cdot z_1\cdot z_2,$$

where: $z_1=(x_2+0.5\cdot x_1-x_{20}'')/(x_{20}'-x_{20}'')$, $z_2=(x_{20}'-x_2-0.5\cdot x_1)/(x_{20}'-x_{20}'')$, x_1, x_2—mole fractions of component (1) and (2), respectively, x_{20}', x_{20}''—values of x_2 on the saturation curve which cuts the $x_1=0$ axis.

All experimental compositions on the saturation curve at 298.2 K (compositions of tie lines were included), Refs. 2 and 5, as well as the ''best'' mutual solubility values of the binary system, Ref. 6, were used in the calculations. The parameters calculated by the least-squares method are: $a_1=-0.319\,92$, $a_2=-0.005\,56$, $a_3=1.107\,75$. The standard error of estimate was 0.0071. The compositions of the saturation curve calculated by the proposed equation at 298.2 K are presented in Table 63 and in Fig. 32.

TABLE 63. Calculated compositons along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 104 Ref. 6	0.3245	0.5200
0.1982	0.0200	0.3149	0.5400
0.2479	0.0400	0.3049	0.5600
0.2828	0.0600	0.2944	0.5800
0.3093	0.0800	0.2835	0.6000
0.3300	0.1000	0.2722	0.6200
0.3464	0.1200	0.2605	0.6400
0.3594	0.1400	0.2484	0.6600
0.3696	0.1600	0.2360	0.6800
0.3774	0.1800	0.2232	0.7000
0.3833	0.2000	0.2101	0.7200
0.3874	0.2200	0.1967	0.7400
0.3900	0.2400	0.1830	0.7600
0.3912	0.2600	0.1689	0.7800
0.3912	0.2800	0.1546	0.8000
0.3901	0.3000	0.1401	0.8200
0.3879	0.3200	0.1252	0.8400
0.3848	0.3400	0.1101	0.8600
0.3809	0.3600	0.0948	0.8800
0.3761	0.3800	0.0792	0.9000
0.3706	0.4000	0.0633	0.9200
0.3645	0.4200	0.0473	0.9400
0.3576	0.4400	0.0310	0.9600
0.3502	0.4600	0.0144	0.9800
0.3421	0.4800	0.0000	0.9972 Ref. 6
0.3336	0.5000		

Phases in equilibrium

The phases in equilibrium were measured also at 293 K, 298 K, and at boiling temperatures at 101.3 kPa. The tie lines cover the whole area of miscibility gap. They are consistent within each data set, as well as with one another. However, the tie lines reported at 298.2 K,[2,5] cross slightly as could be noticed if a large scale graph were plotted. The tie lines are treated as tentative.

The plait point of the system changes with temperature. At 293.2 K it was reported to be $x_1=0.292$, $x_2=0.069$, (Ref. 4) at 298.2 K$-x_1=0.27$, $x_2=0.07$ (Ref. 5) while at 101 kPa at boiling temperature (348.9±0.1 K) it was estimated by the evaluator to be $x_1=0.370\pm0.004$, $x_2=0.209\pm0.001$.

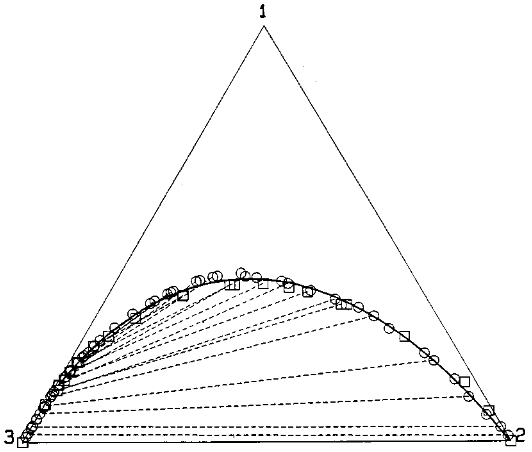

FIG. 32. Phase diagram of the system 2-propanol (1)—toluene (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental results of Ref. 2, □—experimental results of Ref. 5, dashed lines—experimental tie lines, Refs. 2 and 5.

References:

[1]E. Leikola, Suomen Kemistil. B. **13**, 13 (1940).

[2]E. R. Washburn and A. E. Beguin, J. Am. Chem. Soc. **62**, 579 (1940).

[3]L. Stankova, F. Vesely, and J. Pick, Collect. Czech. Chem. Commun. **35**, 1 (1970).

[4]I. A. Borisova, V. G. Vatskova, A. I. Gorbunov, and N. M. Sokolov, Khim. Prom-st (Moscow) 347 (1978).

[5]T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

[6]D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon New York, 1989).

[7]V. V. Kafarov, ed., *Spravochnik po Rastvorimosti*, Vol. 2, Troinye, Mnogokomponentnye Sistemy, Kniga II (Izd. Akademii Nauk SSSR, Moskva, 1963).

[8]K. Hlavaty, Collect. Czech Chem. Commun. **37**, 4005 (1972).

[9]T. M. Letcher, S. Ravindran, and S. E. Radloff, Fluid Phase Equilib. **69**, 251 (1991).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. R. Washburn and A. E. Beguin, J. Am. Chem. Soc. **62**, 579–81 (1940).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/ °C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
25.00	298.15	0.0131	0.0003	0.0425	0.0013
		0.0349	0.0004	0.1076	0.0018
		0.0561	0.0007	0.1650	0.0030
		0.0842	0.0009	0.2340	0.0038
		0.1159	0.0027	0.3016	0.0107
		0.1385	0.0049	0.3438	0.0188
		0.1714	0.0120	0.3944	0.0422
		0.2044	0.0206	0.4364	0.0675
		0.2453	0.0362	0.4753	0.1074
		0.2756	0.0512	0.4957	0.1413
		0.3084	0.0720	0.5101	0.1827
		0.3333	0.0958	0.5117	0.2255
		0.3627	0.1289	0.5089	0.2773
		0.3882	0.1710	0.4961	0.3350
		0.3983	0.2016	0.4814	0.3736
		0.4052	0.2475	0.4559	0.4270
		0.3946	0.2848	0.4255	0.4709
		0.3861	0.3394	0.3905	0.5263
		0.3634	0.4097	0.3430	0.5928
		0.3228	0.5270	0.2745	0.6872
		0.2715	0.6144	0.2176	0.7550
		0.2127	0.7162	0.1597	0.8243
		0.1493	0.8096	0.1064	0.8848
		0.0636	0.9172	0.0431	0.9530

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.00	298.15	0.0136	0.9864	0.0216	0.0000	0.0089	0.9911	0.0687	0.0001
		0.0343	0.9612	0.0400	0.0006	0.0227	0.9764	0.1216	0.0030
		0.1069	0.8592	0.0690	0.0006	0.0745	0.9184	0.1977	0.0028
		0.1942	0.7444	0.0875	0.0012	0.1434	0.8430	0.2414	0.0052
		0.3019	0.5686	0.1102	0.0025	0.2490	0.7190	0.2900	0.0102
		0.3426	0.4696	0.1222	0.0032	0.3062	0.6435	0.3140	0.0125
		0.3805	0.3549	0.1377	0.0038	0.3790	0.5420	0.3434	0.0146
		0.3976	0.2600	0.1570	0.0081	0.4423	0.4435	0.3740	0.0296
		0.3962	0.1934	0.1745	0.0123	0.4857	0.3635	0.3992	0.0433
		0.3859	0.1643	0.1911	0.0165	0.4995	0.3260	0.4210	0.0558
		0.3602	0.1251	0.2087	0.0219	0.5100	0.2716	0.4413	0.0709
		0.3558	0.1200	0.2167	0.0268	0.5105	0.2640	0.4473	0.0847
		0.3396	0.1019	0.2331	0.0311	0.5120	0.2356	0.4650	0.0950

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, as described in Refs. 1, 2, was used. Refractive indexes of mixtures were measured by Abbe refractometer. Binary mixtures of known composition placed in small Erlenmeyer flasks were titrated with water or toluene from weighed pipettes and shaken mechanically in a constant temperature bath. Measured refractive indexes of saturated solutions were plotted for each component. These plots were used further to determine concentration of equilibrium phases. Tie lines were obtained by adding alcohol to water–toluene mixtures and shaking the samples from time to time during the twenty-four hours while they were kept in a constant temperature bath. After separation, refractive indexes of both phase were measured and concentration of each component was read from the plots. The sum of calculated phase concentrations was always equal to 1.0000±0.0001.

Source and Purity of Materials:

(1) Eastman Kodak Company; refluxed with CaO, distilled, middle fraction was used; b.p.=81.7–81.9 °C, $d(25\ °C,4\ °C)=0.780\ 87$, $n(25\ °C,D)=1.3748$.

(2) Eastman Kodak Company; used as received; $n(25\ °C,D)=1.4938$.

(3) distilled over $KMnO_4$.

Estimated Error:

temp. ±0.01 °C.

References:

[1] R. Vold and E. R. Washburn, J. Am. Chem. Soc. **54**, 4217 (1932).

[2] E. R. Washburn and H. C. Spencer, J. Am. Chem. Soc. **56**, 361 (1934).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]

(2) Toluene (methylbenzene); C_7H_8; [108-88-3]

(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. Stankova, F. Vesely, and J. Pick, Collect. Czech. Chem. Commun. 1970, **35**, 1–12.

Variables: $T/K=293-352$

Compiled by: A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/$ °C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
20.00	293.15	0.0301	0.0004	0.0936	0.0017
		0.0445	0.0005	0.1342	0.0024
		0.0721	0.0007	0.2053	0.0029
		0.0981	0.0013	0.2650	0.0053
		0.1225	0.0028	0.3148	0.0111
		0.1453	0.0055	0.3559	0.0206
		0.1667	0.0094	0.3893	0.0338
		0.1865	0.0143	0.4163	0.0490
		0.2050	0.0204	0.4375	0.0668
		0.2219	0.0275	0.4538	0.0861
		0.2756	0.0512	0.4957	0.1413
		0.3039	0.0713	0.5060	0.1821
		0.3366	0.0939	0.5168	0.2211
		0.3432	0.1132	0.5049	0.2554
		0.3548	0.1293	0.5013	0.2802
		0.3696	0.1595	0.4894	0.3237
		0.3936	0.1957	0.4819	0.3674
		0.3919	0.2393	0.4508	0.4220
		0.3909	0.2770	0.4271	0.4641
		0.3870	0.3268	0.3974	0.5145
		0.3703	0.3867	0.3574	0.5723
		0.3399	0.4651	0.3058	0.6416
		0.2910	0.5772	0.2394	0.7281
		0.2501	0.6402	0.1978	0.7762
		0.1992	0.7185	0.1503	0.8311
		0.1322	0.8063	0.0953	0.8914

Compositions along the saturation curve at normal boiling point ($p/kPa=101.32$)

$t/$ °C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
77.25	350.40	0.1517	0.0134	0.3591	0.0486
76.95	350.10	0.1997	0.0297	0.4194	0.0956
76.00	349.15	0.2495	0.0536	0.4615	0.1520
76.75	349.90	0.3193	0.0971	0.4965	0.2314
76.90	350.05	0.3290	0.1097	0.4944	0.2527
76.70	349.85	0.3736	0.1885	0.4706	0.3640
77.00	350.15	0.3732	0.2309	0.4412	0.4185
76.70	349.85	0.3693	0.3063	0.3945	0.5016
76.85	350.00	0.3292	0.4073	0.3188	0.6047
76.75	349.90	0.2597	0.5860	0.2156	0.7460
79.30	352.45	0.2022	0.6842	0.1573	0.8162

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. A binary mixture of known composition (alcohol–hydrocarbon or alcohol–water) and total mass of about 10–15 g placed in thermostat was titrated by the third component from a calibrated microburette until permanent turbidity was formed. The both branches of solubility curve were in mutual agreement. The binodal curve at normal boiling point was measured in a modified Washburn's ebulliometer[1] until the first lasting turbidity by the titration method. Temperatures were recalculated to the pressure of 760 Torr.

Source and Purity of Materials:

(1) source not specified, analytical grade; dried by $CuSO_4$, distilled with 20 vol % of benzene, the middle fraction was used; $n(20\ °C,D) = 1.3771$, $d(20\ °C,4\ °C) = 0.7851$, b.p. = 82.2 °C.
(2) source not specified, technical grade; twice distilled with 10 vol % of propyl alcohol, twice distilled with 10 vol % of 2-butanone; $n(20\ °C,D) = 1.4967$, $d(20\ °C,4\ °C) = 0.8667$, b.p. = 110.6 °C.
(3) distilled.

Estimated Error:

temp. ±0.05 °C (compiler); comp. ±0.01 mL (accuracy of titration).

References:

[1] E. R. Washburn and A. Beguin, J. Am. Chem. Soc. **62**, 579 (1940).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

I. A. Borisova, V. G. Vatskova, A. I. Gorbunov, and N. M. Sokolov, Khim. Prom-st (Moscow) 347 (1978).

Variables:

$T/K = 293/N354$

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/°C$	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
20	293.2	0.0299	0.9502	0.0338	0.0001	0.0200	0.9760	0.1045	0.0005
		0.0530	0.9263	0.0539	0.0001	0.0358	0.9600	0.1595	0.0005
		0.1584	0.8133	0.0906	0.0017	0.1120	0.8820	0.2480	0.0070
		0.2169	0.7226	0.1104	0.0030	0.1615	0.8250	0.2900	0.0120
		0.3320	0.5472	0.1365	0.0050	0.2750	0.6950	0.3400	0.0190
		0.3751	0.4255	0.1506	0.0051	0.3450	0.6000	0.3660	0.0190
		0.3896	0.3519	0.1638	0.0072	0.3870	0.5360	0.3870	0.0260
		0.3946	0.2470	0.1806	0.0115	0.4480	0.4300	0.4100	0.0400
		0.3839	0.1992	0.1998	0.0168	0.4715	0.3750	0.4340	0.0560
		0.2918	0.0692	0.2918	0.0692	0.4950	0.1800	0.4950	0.1800[a]
80.0	353.2	0.0600	0.9031	0.0350	0.0050	0.0412	0.9512	0.1060	0.0232[b]
79.0	352.2	0.0920	0.8559	0.0440	0.0050	0.0648	0.9242	0.1307	0.0228[b]
78.0	351.2	0.1570	0.7632	0.0581	0.0060	0.1162	0.8661	0.1669	0.0265[b]
77.0	350.2	0.2149	0.6821	0.0800	0.0100	0.1664	0.8097	0.2174	0.0416[b]
76.0	349.2	0.3370	0.4671	0.1631	0.0220	0.3031	0.6441	0.3697	0.0765[b]
75.8	349.0	0.3775	0.3077	0.2421	0.0580	0.4000	0.5000	0.4476	0.1645[b]
75.7	348.9	0.3742	0.2098	0.3681	0.2082	0.4560	0.3920	0.4520	0.3920[a,b,c]

[a] Critical solubility point.
[b] Temperatures are the boiling temperatures of the two-phase mixtures.
[c] Boiling temperature estimated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

The method of description of concentration of phases in equilibrium was the same as reported in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified; properties were in agreement with literature data.
(2) source not specified; properties were in agreement with literature data.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] A. S. Mozzhukhin, L. A. Serafimov, and V. A. Mitropolskaya, Zh. Fiz. Khim. **41**, 1687 (1967).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.091	0.001	0.249	0.004
		0.138	0.005	0.343	0.019
		0.193	0.019	0.421	0.064
		0.255	0.049	0.473	0.139
		0.298	0.083	0.488	0.208
		0.353	0.154	0.479	0.320
		0.378	0.247	0.435	0.436
		0.371	0.362	0.369	0.552
		0.329	0.500	0.287	0.668
		0.252	0.656	0.196	0.782
		0.142	0.834	0.099	0.896
		0.073	0.918	0.049	0.949
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hyrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.330	0.488	0.125	0.008	0.291	0.661	0.315	0.031
		0.360	0.405	0.150	0.010	0.342	0.591	0.360	0.037
		0.380	0.305	0.170	0.012	0.403	0.496	0.392	0.042
		0.377	0.238	0.192	0.016	0.440	0.426	0.423	0.054
		0.351	0.154	0.230	0.030	0.477	0.321	0.462	0.092

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; d=0.781 51, n=1.3752.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) 1-Heptene; C_7H_{14} ; [592-76-7]
(3) Water; H_2O; [7732 -18-5]

Original Measurements:

T. M. Letcher, B. C. Bricknell, J. D. Sewery, and S. E. Radloff, J. Chem. Eng. Data **39**, 320–3 (1994).

Variables:

T/K=298

Compiled by:

A. Skrzecz

6.6. 2-Propanol + Water + 1-Heptene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.000	1.000	0.000	1.000
		0.184	0.773	0.126	0.865
		0.281	0.632	0.210	0.771
		0.365	0.468	0.309	0.648
		0.407	0.330	0.397	0.526
		0.417	0.227	0.466	0.415
		0.402	0.145	0.519	0.306
		0.378	0.084	0.559	0.203
		0.349	0.050	0.571	0.134
		0.273	0.021	0.526	0.066
		0.242	0.011	0.500	0.037
		0.059	0.005	0.170	0.023
		0.027	0.001	0.084	0.005
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hyrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.390	0.595	0.412	0.270	0.285	0.711	0.434	0.465
		0.372	0.450	0.412	0.185	0.321	0.633	0.493	0.362
		0.342	0.518	0.382	0.092	0.278	0.688	0.554	0.218
		0.291	0.616	0.300	0.032	0.220	0.759	0.543	0.095
		0.190	0.764	0.197	0.009	0.131	0.860	0.438	0.033

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods have been described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) Aldrich; distilled; purity >99.8 mole % by glc, ρ =0.692 65 g cm^{-3}.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) 2-Propanol (isopropanol isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Heptane (*n*-heptane); C_7H_{16} ; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.05)

6.7. 2-Propanol + Water + Heptane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-propanol–heptane–water is given in Table 64.

TABLE 64. Summary of experimental data for the system 2-propanol–heptane–water

Author(s)	T/K	Type of data[a]	Ref.
Vorobeva and Karapetyants, 1967	298	sat. (14), eq. (10)	1
Letcher *et al.*, 1986	298	sat. (8), eq. (3)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 2-propanol–heptane–water forms a large miscibility gap of type 1 covering the majority of the concentration triangle. Only the heptane–water binary system forms a miscibility gap. The data of this binary system were compiled and critically evaluated in a previously published SDS volume.[3] The recommended mutual solubilities of the binary system heptane–water at 298.2 K[3] are $x_2''=4.3\cdot 10^{-7}$ and $x_3'=5.6\cdot 10^{-4}$. Solubility of water in heptane, $x_3'=5.5\cdot 10^{-3}$, reported by Vorobeva and Karapetyants[1] is 10 times higher but it is consistent with the accuracy of experiments -0.001 mass fraction. A heptane free point on the saturation curve ($x_1=0.049$) in the data of Letcher *et al.*[2] ought to be treated as an artifact of the experimental accuracy. The data are not sufficiently accurate to describe the regions of low concentration of 2-propanol. All compositions of coexisting phases in equilibrium in both data sets are consistent with independently measured saturation curve and with one another. The data of Lecher *et al.*, Ref. 2, show slightly larger solubility for the heptane-poor phase in the region of $x_2=0.2$–0.4. The maximum of 2-propanol concentration is observed on saturation curve which at 298.2 K reaches $x_1=0.46\pm 0.01$ and $x_2=0.18\pm 0.02$ mole fraction. All experimental solubility and equilibrium data reported at 298.2 K were used for calculation of saturation curve. (Water-rich and hydrocarbon-rich branches were treated together.) These data were described by the equation:

$$x_1=0.651\,25+0.083\,32\ln(x_2)-0.261\,69x_2-0.404\,01x_2^2.$$

The least-squares method was used and the standard error of estimate was 0.0186. The equation describes the saturation curve for $x_2<0.91$ mole fraction. The compositions on the saturation curve, calculated by the proposed equation are presented in Table 65 for the selected concentrations of heptane in the mixture and in Fig. 33 as calculated binodal curve (solid line).

TABLE 65. Calculated compositons along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	$4.3\cdot 10^{-7}$ Ref. 6	0.3807	0.4600
0.0754	0.0010	0.3714	0.4800
0.2649	0.0100	0.3616	0.5000
0.3199	0.0200	0.3514	0.5200
0.3719	0.0400	0.3408	0.5400
0.3997	0.0600	0.3297	0.5600
0.4173	0.0800	0.3182	0.5800
0.4292	0.1000	0.3062	0.6000
0.4374	0.1200	0.2939	0.6200
0.4429	0.1400	0.2811	0.6400
0.4463	0.1600	0.2679	0.6600
0.4482	0.1800	0.2544	0.6800
0.4487	0.2000	0.2404	0.7000
0.4480	0.2200	0.2260	0.7200
0.4463	0.2400	0.2113	0.7400
0.4437	0.2600	0.1961	0.7600
0.4402	0.2800	0.1806	0.7800
0.4361	0.3000	0.1647	0.8000
0.4312	0.3200	0.1485	0.8200
0.4257	0.3400	0.1318	0.8400
0.4196	0.3600	0.1148	0.8600
0.4128	0.3800	0.0974	0.8800
0.4056	0.4000	0.0797	0.9000
0.3978	0.4200	0.0000	0.999 44 Ref. 6
0.3895	0.4400		

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 2-propanol–heptane–water were reported in both references at the same temperature 298 K. A plait point of liquid–liquid equilibrium obtained graphically by Vorobeva and Karapetyants[1] was $x_1 = 0.440$ and $x_2 = 0.279$. The tie lines of Ref. 1 cover the whole range of miscibility gap, while only three tie lines of Ref. 2 cover the middle region of miscibility gap $0.1 < x_1 < 0.27$. The compositions of phases in equilibrium reported in Refs. 1 and 2 are consistent. The system behavior, calculated saturation curve as well as the experimental data are presented in Fig. 33.

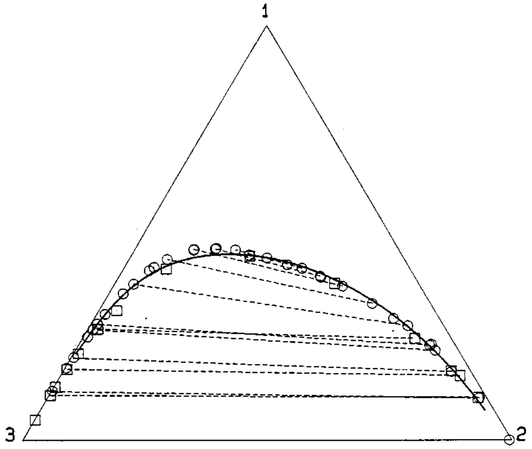

FIG. 33. Phase diagram of the system 2-propanol (1)—heptane (2)—water (3) at 298.2 K. Solid line—calculated saturation curve, ○—experimental data, Ref. 1, □—experimental data, Ref. 2, dashed lines—experimental tie lines, Refs. 1 and 2.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1984 (1967).

[2] T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Heptane (*n*-heptane); C_7H_{16} ; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1984–9 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 1061–3 (1967)].

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9945	0.000	0.999
		0.2315	0.7202	0.160	0.830
		0.2940	0.6119	0.219	0.760
		0.3932	0.4129	0.345	0.604
		0.4236	0.3287	0.405	0.524
		0.4467	0.2397	0.475	0.425
		0.4629	0.1637	0.546	0.322
		0.4584	0.1200	0.584	0.255
		0.4168	0.0598	0.619	0.148
		0.4091	0.0538	0.620	0.136
		0.3540	0.0281	0.604	0.080
		0.3043	0.0160	0.569	0.050
		0.2494	0.0079	0.514	0.027
		0.1740	0.0020	0.410	0.008

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hyrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25	298.2	0.101	0.883	0.119	0.001	0.064	0.933	0.310	0.004
		0.165	0.795	0.200	0.004	0.110	0.882	0.450	0.014
		0.216	0.736	0.267	0.010	0.148	0.842	0.533	0.034
		0.229	0.718	0.281	0.012	0.159	0.830	0.547	0.040
		0.276	0.650	0.377	0.038	0.200	0.784	0.612	0.104
		0.330	0.550	0.436	0.077	0.257	0.715	0.614	0.180
		0.372	0.468	0.460	0.120	0.310	0.650	0.585	0.255
		0.396	0.410	0.461	0.163	0.348	0.601	0.545	0.322
		0.415	0.363	0.459	0.205	0.382	0.557	0.509	0.379
		0.440	0.279	0.440	0.279	0.445	0.470	0.445	0.470[a]

[a] Critical point obtained graphically by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods were described in Ref. 1. Water impurities in alcohol were taken into account in the measurements. Critical point of liquid–liquid equilibrium was obtained graphically by the method reported in Ref. 2.

Source and Purity of Materials:

(1) source and method of preparation were reported in Ref. 1.
(2) source not specified; pure grade; distilled; water concentration was analyzed by the Karl Fischer method.
(3) doubly distilled.

Estimated Error:

Not specified.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[2] E. F. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Heptane (*n*-heptane); C_7H_{16} ; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037-42 (1986).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.049	0.000	0.147	0.000
		0.128	0.002	0.326	0.009
		0.209	0.009	0.456	0.033
		0.313	0.035	0.552	0.103
		0.413	0.087	0.583	0.205
		0.444	0.242	0.472	0.429
		0.378	0.449	0.321	0.635
		0.167	0.793	0.111	0.881

Compositions of coexisting phases

t/°C (compiler)	T/K	x'_1 hydrocarbon-rich phase	x'_2	x''_1 water-rich phase	x''_2	w'_1 hydrocarbon-rich phase (compiler)	w'_2	w''_1 water-rich phase (compiler)	w''_2
25	298.2	0.245	0.680	0.268	0.019	0.175	0.809	0.522	0.062
		0.155	0.817	0.171	0.005	0.102	0.893	0.401	0.020
		0.102	0.880	0.108	0.002	0.065	0.932	0.286	0.009

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) Aldrich, Gold label, 99.5 mole %; dried with potassium carbonate, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1] S. W. Briggs and E. W. Commings, Ind. Eng. Chem. **35**, 411 (1943).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) *m*-Xylene (1,3-dimethylbenzene, 1,3-xylene); C_8H_{10} ; [108-38-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

6.8. 2-Propanol + Water + *m*-Xylene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.091	0.001	0.249	0.005
		0.139	0.002	0.347	0.009
		0.195	0.010	0.432	0.039
		0.261	0.028	0.498	0.094
		0.322	0.078	0.503	0.215
		0.367	0.139	0.482	0.323
		0.391	0.221	0.436	0.435
		0.390	0.330	0.369	0.552
		0.353	0.466	0.287	0.669
		0.276	0.625	0.196	0.783
		0.157	0.806	0.099	0.894
		0.085	0.899	0.051	0.946
		0.000	0.997	0.000	0.999

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1 hydrocarbon-rich phase	x'_2	x''_1 water-rich phase	x''_2	w'_1 hydrocarbon-rich phase (compiler)	w'_2	w''_1 water-rich phase (compiler)	w''_2
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.031	0.953	0.089	0.001	0.018	0.979	0.245	0.005
		0.134	0.823	0.129	0.002	0.084	0.908	0.328	0.009
		0.286	0.588	0.192	0.009	0.210	0.762	0.429	0.036
		0.366	0.407	0.234	0.020	0.317	0.624	0.475	0.072
		0.383	0.207	0.322	0.072	0.439	0.420	0.510	0.202

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; $d=0.781\ 51$, $n=1.3752$.
(2) BDH; used as received; purity better than 99.6 mole % by glc; $d=0.860\ 32$, $n=1.54946$.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) *o*-Xylene (1,2-dimethylbenzene, 1,2-xylene); C_8H_{10}; [95-47-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

$T/K=298$

Compiled by:

A. Skrzecz

6.9. 2-Propanol + Water + *o*-Xylene

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.091	0.001	0.249	0.005
		0.139	0.003	0.346	0.013
		0.195	0.011	0.431	0.043
		0.260	0.031	0.493	0.104
		0.319	0.077	0.501	0.214
		0.356	0.134	0.477	0.317
		0.386	0.219	0.433	0.434
		0.386	0.328	0.367	0.551
		0.351	0.463	0.287	0.668
		0.274	0.620	0.196	0.782
		0.158	0.804	0.099	0.893
		0.084	0.899	0.050	0.947
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
$t/°C$	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.046	0.938	0.086	0.001	0.027	0.970	0.238	0.005
		0.098	0.867	0.118	0.002	0.060	0.934	0.306	0.009
		0.293	0.577	0.206	0.014	0.217	0.754	0.443	0.053
		0.364	0.422	0.208	0.034	0.310	0.635	0.420	0.121
		0.381	0.204	0.335	0.092	0.440	0.416	0.501	0.243

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2; purity better than 99.6 mole % by glc; $d = 0.781\,51$, $n = 1.3752$.
(2) BDH; used as received; purity better than 99.6 mole % by glc; $d = 0.875\,88$, $n = 1.5029$.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053–60 (1989).

Variables:

T/K = 298

Compiled by:

A. Skrzecz

6.10. 2-Propanol + Water + *p*-Xylene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.998	0.000	0.9997
		0.083	0.892	0.050	0.946
		0.158	0.806	0.099	0.894
		0.277	0.627	0.196	0.784
		0.354	0.468	0.287	0.670
		0.391	0.332	0.369	0.553
		0.394	0.223	0.436	0.436
		0.366	0.138	0.483	0.321
		0.321	0.078	0.502	0.216
		0.273	0.039	0.498	0.126
		0.259	0.032	0.490	0.107
		0.195	0.011	0.431	0.043
		0.129	0.002	0.328	0.009
		0.050	0.001	0.149	0.005
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.345	0.102	0.220	0.017	0.499	0.261	0.460	0.063
		0.399	0.268	0.178	0.010	0.410	0.487	0.405	0.040
		0.349	0.480	0.128	0.005	0.280	0.679	0.323	0.022
		0.265	0.648	0.075	0.002	0.185	0.797	0.211	0.010
		0.165	0.797	0.043	0.000	0.104	0.889	0.130	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. A binary mixture of known composition was titrated with the third component until cloudiness was observed. Tie line compositions were related to the coexistence curve; water was determined by the Karl Fischer titration. The methods were described in Ref. 1.

Source and Purity of Materials:

(1) source not specified; used as received.
(2) source not specified; recrystallized three times.
(3) not specified.

Estimated Error:

comp. <0.005 mole fraction (estimated authors' precision on binodal curve), <0.01 mole fraction (estimated authors' precision of tie lines).

References:

[1]T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Ethylbenzene (phenylethane); C_8H_{10}; [100-41-4]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. T. Knypl and S. Z. Wojdylo, J. Appl. Chem. **17**, 361–3 (1967).

Variables:

T/K=298

Compiled by:

A. Skrzecz

6.11. 2-Propanol + Water + Ethylbenzene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.15	0.0681	0.0036	0.1930	0.0180
		0.0690	0.0002	0.1980	0.0010
		0.1056	0.0003	0.2823	0.0015
		0.1186	0.0102	0.2982	0.0454
		0.1304	0.0023	0.3305	0.0105
		0.1482	0.0032	0.3630	0.0140
		0.1784	0.0071	0.4100	0.0290
		0.2278	0.0179	0.4692	0.0651
		0.3194	0.0652	0.5160	0.1860
		0.3751	0.1270	0.5010	0.2996
		0.3974	0.2012	0.4551	0.4071
		0.3992	0.2737	0.4070	0.4930
		0.3785	0.3931	0.3316	0.6084
		0.1656	0.8129	0.1030	0.8930

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.15	0.0175	0.9825	0.0348	0.0006	0.010	0.990	0.107	0.003
		0.0535	0.9465	0.0624	0.0008	0.031	0.969	0.181	0.004
		0.1189	0.8646	0.0888	0.0012	0.072	0.925	0.244	0.006
		0.1753	0.7982	0.1137	0.0015	0.110	0.885	0.298	0.007
		0.2824	0.6234	0.1484	0.0035	0.200	0.780	0.363	0.015
		0.3356	0.5327	0.1766	0.0086	0.255	0.715	0.405	0.035
		0.3928	0.4172	0.2276	0.0179	0.331	0.621	0.469	0.065
		0.3961	0.2990	0.2790	0.0391	0.390	0.520	0.505	0.125
		0.3927	0.1927	0.3119	0.0565	0.458	0.397	0.519	0.166
		0.3657	0.1033	0.3657	0.1033	0.517	0.258	0.517	0.258[a]

[a]Critical point of solubility.

Auxiliary Information

Method/Apparatus/Procedure:

The saturation isotherm was obtained by cloud-point titration method. Liquid–liquid equilibrium was determined by the synthetic method. Physical properties of phases in equilibrium, refractive index and density, were measured and compositions were found from relationships obtained in the isothermal measurements.

Source and Purity of Materials:

(1) Chemical Works ‘‘Oswiecim’’ (Poland), laboratory grade; used as received; $d(20\ °C, 4\ °C) = 0.7864$, $n(20\ °C, D) = 1.3768$.
(2) Chemical Works ‘‘Oswiecim’’ (Poland), laboratory grade; used as received; $d(20\ °C, 4\ °C) = 0.8665$, $n(20\ °C, D) = 1.4958$.
(3) distilled.

Estimated Error:

temp. ±0.05 °C (estimated by the compiler).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) 1,7-Octadiene; C_8H_{14}; [3710-30-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. O. Emelyanov, L. V. Melnik, and B. N. Bobylev, Zh. Prikl. Khim. (Leningrad) **64**, 1700–4 (1991). [Eng. transl. Russ. J. Appl. Chem. (Leningrad) **64**, 1555–8 (1991)].

Variables:

T/K = 293–360

Compiled by:

A. Skrzecz

6.12. 2-Propanol + Water + 1,7-Octadiene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
25.00	293.15	0.0000	0.0003	0.0000	0.0018
		0.2325	0.0045	0.4952	0.0176
		0.3765	0.0668	0.5654	0.1840
		0.4010	0.1155	0.5292	0.2795
		0.4099	0.1787	0.4761	0.3806
		0.4103	0.2466	0.4250	0.4684
		0.3904	0.3632	0.3454	0.5892
		0.2874	0.6409	0.1936	0.7919
		0.1453	0.8351	0.0864	0.9101
		0.0000	0.9998	0.0000	0.99997
87.00	360.15	0.0000	0.0149	0.0000	0.0847
		0.0000	0.9995	0.0000	0.99992

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
20.00	293.15	0.0366	0.9595	0.0490	0.0005	0.0204	0.9790	0.1463	0.0027
		0.1115	0.8736	0.1045	0.0005	0.0649	0.9325	0.2796	0.0025
		0.1687	0.8052	0.1368	0.0005	0.1021	0.8932	0.3452	0.0023
		0.2415	0.7097	0.1792	0.8199	0.1551	0.8356	0.1065	0.8934
		0.2849	0.6449	0.2066	0.0019	0.1914	0.7945	0.4618	0.0078
		0.3342	0.5439	0.2407	0.0032	0.2443	0.7290	0.5086	0.0124
		0.3681	0.4404	0.2865	0.0098	0.2985	0.6549	0.5559	0.0349
		0.3898	0.3647	0.3062	0.0217	0.3443	0.5907	0.5593	0.0727
		0.4000	0.1130	0.4000	0.1130	0.5311	0.2751	0.5311	0.2751

Auxiliary Information

Method/Apparatus/Procedure:

Mutual solubility was determined by the standard isothermic titration method until turbidity was observed. Phase equilibrium was measured in the thermostated separator. Concentrations of 2-propanol and 1,7-octadiene in the equilibrium phases were determined by the glc analysis (FID detector). Water was analyzed by the Karl Fischer method.

Source and Purity of Materials:

(1) source not specified, pure grade; dried, distilled; b.p. = 355.54 K.
(2) synthesized in the laboratory; distilled; purity >99.5%; b.p. = 390.65 K.
(3) doubly distilled.

Estimated Error:

Not reported.

Components:
(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
N. Arda and A. A. Sayar, Fluid Phase Equilib. **73,** 129–38 (1992).

Variables:
T/K=293

Compiled by:
A. Skrzecz

6.13. 2-Propanol + Water + 2,2,4-Trimethylpentane

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	293.2	0.0000	0.0004	0.0000	0.0028
		0.0044	0.0010	0.0145	0.0060
		0.0126	0.0015	0.0406	0.0094
		0.0380	0.0022	0.1152	0.0125
		0.0541	0.0027	0.1582	0.0151
		0.0673	0.0038	0.1907	0.0207
		0.0969	0.0038	0.2593	0.0193
		0.1074	0.0044	0.2811	0.0218
		0.1313	0.0044	0.3292	0.0210
		0.1641	0.0056	0.3874	0.0251
		0.1965	0.0070	0.4380	0.0297
		0.2138	0.0076	0.4632	0.0312
		0.2471	0.0082	0.5086	0.0320
		0.3077	0.0163	0.5684	0.0573
		0.3364	0.0222	0.5893	0.0739
		0.3921	0.0380	0.6173	0.1137
		0.4151	0.0489	0.6208	0.1389
		0.4306	0.0613	0.6156	0.1667
		0.4401	0.0838	0.5930	0.2147
		0.4467	0.1031	0.5744	0.2521
		0.4392	0.1333	0.5351	0.3088
		0.4283	0.1496	0.5104	0.3388
		0.4385	0.1615	0.5067	0.3547
		0.4355	0.2121	0.4612	0.4269
		0.4102	0.2588	0.4096	0.4913
		0.3916	0.3179	0.3616	0.5580
		0.3389	0.4632	0.2650	0.6886
		0.2737	0.5775	0.1933	0.7752
		0.0995	0.8318	0.0585	0.9294
		0.0478	0.8823	0.0274	0.9606
		0.0000	0.9519	0.0000	0.9921

Compositions of coexisting phase

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	293.2	0.3752	0.3983	0.3595	0.0266	0.3126	0.6308	0.6051	0.0852
		0.3207	0.4931	0.3199	0.0172	0.2441	0.7134	0.5802	0.0594
		0.2851	0.5706	0.2709	0.0124	0.2018	0.7676	0.5320	0.0461
		0.2517	0.6497	0.2337	0.0080	0.1660	0.8145	0.4908	0.0319
		0.2094	0.6888	0.2079	0.0082	0.1352	0.8451	0.4535	0.0339
		0.1761	0.7329	0.1684	0.0056	0.1103	0.8726	0.3947	0.0251
		0.1691	0.7342	0.1499	0.0064	0.1061	0.8757	0.3613	0.0293
		0.1489	0.7587	0.1277	0.0060	0.0920	0.8909	0.3202	0.0288
		0.1152	0.7848	0.0985	0.0057	0.0704	0.9113	0.2607	0.0285
		0.1022	0.8078	0.0867	0.0040	0.0614	0.9224	0.2363	0.0207
		0.0672	0.8481	0.0518	0.0029	0.0394	0.9457	0.1521	0.0164
		0.0562	0.8623	0.0430	0.0029	0.0327	0.9531	0.1287	0.0162
		0.0378	0.8903	0.0277	0.0019	0.0216	0.9661	0.0859	0.0110
		0.0198	0.9104	0.0140	0.0004	0.0112	0.9770	0.0450	0.0022

Auxiliary Information

Method/Apparatus/Procedure:

Solubility measurements were made in an equilibrium cell with a stirrer[1] by titration of binary mixtures of known composition with the third component. This was done using 2-propanol for heterogeneous hydrocarbon–water mixtures, until the turbidity had disappeared and 2,2,4-trimethylpentane for homogeneous alcohol–water mixtures until cloudiness was observed. Tie lines were measured in the same cell filled with ternary heterogeneous mixtures of known composition. Mixtures were stirred for 1 h and after separation the samples of each phase were twice analyzed; 2-propanol concentration was determined by glc using Supelco Carbopack-C 0.2%, CW-1500, 60/80 column on Aerograph Hydrogen-Flame, Model 600-C (N_2, 12–13 mL/s, 373 K). Water was determined by the Karl Fischer method.

Source and Purity of Materials:

(1) Merck; dried over anhydrous K_2CO_3, distilled, with the middle 80% collected; impurities <0.1% by glc; b.p.=355.7 ±0.1 K, n(293 K,D)=1.3756±0.0005, ρ(293 K)=783.2 ±0.1 kg m^{-3}.
(2) Merck; dried over anhydrous K_2CO_3, distilled, with the middle 60% collected; impurities <0.2% by glc; b.p.=372.9 ±0.1 K, n(293 K,D)=1.3890±0.0005, ρ(293 K)=695.8 ±0.1 kg m^{-3}.
(3) not specified.

Estimated Error:

temp. ±0.1 K; solubility curve ±0.0025 mass fraction, analysis: 2-propanol ±0.0050 mass fraction, water ±0.0025 mass fraction.

References:

[1] A. A. Sayar, J. Chem. Eng. Data **36**, 61 (1991).

Components:	**Original Measurements:**
(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0] (2) Octane (*n*-octane); C_8H_{18}; [111-65-9] (3) Water; H_2O; [7732-18-5]	A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1984–9 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 1061–3 (1967)].
Variables: T/K=298	**Compiled by:** A. Skrzecz

6.14. 2-Propanol + Water + Octane

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9937	0.000	0.999
		0.0870	0.9069	0.048	0.951
		0.2299	0.7164	0.143	0.847
		0.3690	0.4957	0.273	0.697
		0.4511	0.3252	0.397	0.544
		0.4858	0.2311	0.481	0.435
		0.5047	0.1610	0.554	0.336
		0.4984	0.0953	0.622	0.226
		0.4792	0.0672	0.645	0.172
		0.4388	0.0418	0.651	0.118
		0.3993	0.0272	0.641	0.083
		0.3472	0.0158	0.611	0.053
		0.2760	0.0066	0.548	0.025
		0.1796	0.0014	0.420	0.006

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25	298.2	0.055	0.933	0.1404	0.0004	0.030	0.968	0.352	0.002
		0.163	0.803	0.2925	0.0076	0.096	0.898	0.566	0.028
		0.230	0.716	0.4106	0.0308	0.143	0.847	0.645	0.092
		0.281	0.643	0.4606	0.0532	0.184	0.801	0.651	0.143
		0.313	0.598	0.4809	0.0711	0.212	0.770	0.641	0.180
		0.411	0.435	0.5050	0.1551	0.320	0.644	0.560	0.327
		0.448	0.349	0.4919	0.2170	0.382	0.566	0.496	0.416
		0.464	0.306	0.4804	0.2549	0.416	0.522	0.460	0.464
		0.473	0.282	0.473	0.282	0.437	0.495	0.437	0.495[a]

[a] Critical point obtained graphically by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods were described graphically in Ref. 1. Water impurity in alcohol were taken into account in the measurements. Critical point of liquid–liquid equilibrium was obtained graphically by the method reported in Ref. 2.

Source and Purity of Materials:

(1) source and method of preparation were reported in Ref. 1.
(2) source not specified; pure grade; distilled; water concentration was analyzed by the Karl Fischer method.
(3) doubly distilled.

Estimated Error:

Not specified.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[2] E. F. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Mesitylene (1,3,5 -trimethylbenzene); C_9H_{12} ; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

$T/\text{K}=298$

Compiled by:

A. Skrzecz

6.15. 2-Propanol + Water + Mesitylene

Experimental Data

Compositions along the saturation curve

$t/°\text{C}$	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.069	0.000	0.198	0.000
		0.113	0.001	0.297	0.005
		0.166	0.005	0.391	0.024
		0.229	0.014	0.473	0.058
		0.326	0.044	0.541	0.146
		0.389	0.093	0.533	0.255
		0.410	0.138	0.499	0.336
		0.415	0.207	0.440	0.439
		0.403	0.303	0.367	0.552
		0.370	0.433	0.286	0.669
		0.297	0.595	0.195	0.783
		0.174	0.783	0.099	0.893
		0.093	0.888	0.050	0.947
		0.000	0.999	0.000	0.9998

Compositions of coexisting phase

		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
$t/°\text{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.187	0.763	0.188	0.008	0.108	0.883	0.422	0.036
		0.270	0.640	0.270	0.027	0.171	0.812	0.505	0.101
		0.330	0.525	0.332	0.047	0.232	0.738	0.542	0.154
		0.387	0.380	0.390	0.096	0.318	0.625	0.530	0.261

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by refluxing with Mg and I_2 ; purity better than 99.6 mole % by glc; $d=0.781\,51$, $n=1.3752$.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs, and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 2-Propanol (isopropanol, isopropyl alcohol); C_3H_8O; [67-63-0]
(2) Nonane (*n*-nonane); C_9H_{20} ; [111-84-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **41**, 1984–9 (1967). [Eng. transl. Russ. J. Phys. Chem. **41**, 1061-3 (1967)].

Variables:

T/K=298

Compiled by:

A. Skrzecz

6.16. 2-Propanol + Water + Nonane

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.0000	0.9929	0.000	0.999
		0.1443	0.8301	0.075	0.921
		0.2908	0.6367	0.174	0.813
		0.4147	0.4446	0.295	0.675
		0.4623	0.3582	0.361	0.597
		0.4877	0.3134	0.401	0.550
		0.5232	0.2274	0.483	0.448
		0.5451	0.1572	0.562	0.346
		0.5432	0.0933	0.638	0.234
		0.5287	0.0682	0.665	0.183
		0.5084	0.0525	0.676	0.149
		0.4701	0.0340	0.680	0.105
		0.3706	0.0123	0.637	0.045
		0.2817	0.0047	0.557	0.020
		0.1666	0.0006	0.399	0.003

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25	298.2	0.092	0.888	0.194	0.001	0.046	0.951	0.443	0.005
		0.152	0.816	0.334	0.009	0.080	0.915	0.608	0.034
		0.177	0.786	0.389	0.015	0.095	0.899	0.649	0.053
		0.219	0.733	0.449	0.027	0.122	0.870	0.676	0.088
		0.291	0.637	0.519	0.060	0.174	0.813	0.671	0.166
		0.350	0.547	0.545	0.099	0.226	0.754	0.632	0.244
		0.374	0.516	0.546	0.120	0.248	0.730	0.605	0.284
		0.415	0.445	0.546	0.152	0.295	0.675	0.568	0.338
		0.452	0.385	0.541	0.192	0.342	0.621	0.525	0.397
		0.465	0.363	0.537	0.206	0.360	0.600	0.510	0.417
		0.490	0.311	0.521	0.242	0.404	0.547	0.470	0.466
		0.507	0.279	0.507	0.279	0.435	0.510	0.435	0.510[a]

[a] Critical point obtained graphically by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods were described in Ref. 1. Water impurities in alcohol were taken into account in the measurements. Critical point of liquid–liquid equilibrium was obtained graphically by the method reported in Ref. 2.

Source and Purity of Materials:

(1) source and method of preparation were reported in Ref. 1.
(2) source not specified; pure grade; distilled; water concentration was analyzed by the Karl Fischer method.
(3) doubly distilled.

Estimated Error:

Not specified.

References:

[1] A. I. Vorobeva and M. Kh. Karapetyants, Zh. Fiz. Khim. **40**, 3018 (1966).
[2] E. F. Zilberman, Zh. Fiz. Khim. **26**, 1458 (1952).

7. 2-Methyl-1-propanol+Water

Components:

(1) 2-Methyl-1-propanol (isobutanol, isobutyl alcohol); $C_4H_{10}O$; [78–83-1]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.05)

7.1. 2-Methyl-1-propanol + Water + Benzene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-methyl-1-propanol–benzene–water is given in Table 66.

TABLE 66. Summary of experimental data for the system 2-methyl-1-propanol–benzene–water

Author(s)	T/K	Type of data[a]	Ref.
Alberty and Washbum, 1945	298	sat. (14), eq. (10)	1
Letcher *et al.*, 1990	298	sat. (13), eq. (4)	2

[a] Number of experimental points in parentheses.

The ternary system 2-methyl-1-propanol–benzene–water forms a miscibility gap of type 2. Two binary systems, benzene–water and 2-methyl-1-propanol–water, form miscibility gaps. These binary systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. These recommended values of mutual solubility at 298 K are $x_2'=0.9970$, $x_2''=0.000\,409$ for benzene–water system, and $x_1'=0.548$, $x=0.021$ for 2-methyl-1-propanol–water system. The tie lines and experimental points along the saturation curve reported by Alberty and Washburn[1] are consistent with one another. The reported mutual solubility of the 2-methyl-1-propanol–water system, $x_1'=0.5425$ and $x_1''=0.0208$ are in good agreement with the recommended values. Data of Letcher *et al.*[2] were reported in graphical form only and therefore are not compiled. The maximum alcohol concentration on the binodal curve at 298 K, $x_1=0.55$,[1] is consistent with the results of Alberty and Washburn,[1] $x_1=0.558$. The experimental tie lines at 298.2 K, Ref. 1, are presented in Fig. 34 together with the experimental points along the saturation curve.

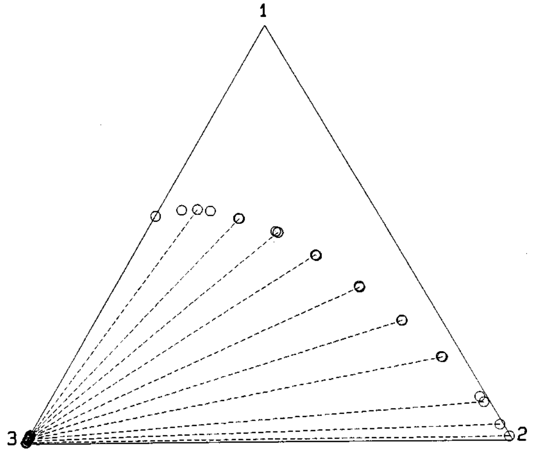

FIG. 34. Phase diagram of the system 2-methyl-1-propanol (1)—benzene (2)—water (3) at 298.2 K. ○—experimental results of Ref. 1, dashed lines—experimental tie lines, Ref. 1.

References:

[1] R. A. Alberty and E. R. Washburn, J. Phys. Chem. **49**, 4 (1945).
[2] T. M. Letcher, J. Sewry, and S. Radloff, S. Afr. J. Chem. **43**, 56 (1990).
[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).
[4] A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York 1984).

Components:

(1) 2-Methyl-1-propanol (isobutanol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. A. Alberty and E. R. Washburn, J. Phys. Chem. **49**, 4–8 (1945).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.2	0.1050	0.8796	0.1014	0.8950
		0.2015	0.7530	0.2003	0.7887
		0.2890	0.6286	0.2975	0.6819
		0.3714	0.5011	0.3992	0.5675
		0.4450	0.3781	0.5020	0.4495
		0.5038	0.2662	0.5996	0.3339
		0.5361	0.1742	0.6785	0.2324
		0.5543	0.1073	0.7394	0.1509
		0.5564	0.0471	0.7922	0.0706
		0.5425	0.0000	0.8299	0.0000
		0.0208	0.0000	0.0802	0.0000
		0.0156	0.0004	0.0610	0.0017
		0.0101	0.0006	0.0402	0.0026
		0.0051	0.0005	0.0205	0.0023

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25.0	298.2	0.0097	0.9873	0.0023	0.0005	0.0092	0.9901	0.0093	0.0020
		0.0377	0.9541	0.0058	0.0007	0.0361	0.9620	0.0233	0.0028
		0.0917	0.8946	0.0091	0.0006	0.0884	0.9084	0.0362	0.0027
		0.2002	0.7559	0.0108	0.0006	0.1987	0.7907	0.0430	0.0026
		0.2874	0.6303	0.0122	0.0005	0.2958	0.6836	0.0482	0.0020
		0.3681	0.5040	0.0133	0.0004	0.3957	0.5709	0.0523	0.0018
		0.4465	0.3751	0.0146	0.0003	0.5044	0.4466	0.0573	0.0014
		0.5014	0.2718	0.0154	0.0003	0.5948	0.3398	0.0604	0.0013
		0.5355	0.1761	0.0164	0.0003	0.6768	0.2346	0.0643	0.0011
		0.5580	0.0788	0.0188	0.0001	0.7651	0.1139	0.0732	0.0004

Auxiliary Information

Method/Apparatus/Procedure:

The titration method as in Ref. 1 was used. 50 mL flasks with dry stoppers were used for titration. Evaporation was monitored and was usually less than 0.0002 of the mass. Samples were shaken during titration and a titrant was added in drops (water drops weighed 5–7 mg, alcohol and benzene drops weighed 2–4 mg). An Abbe refractometer was used to measure the refractive indexes of the saturated solutions. Results were plotted for each component separately. Tie-lines were determined from the mixtures of equal volume, which were equilibrated for 4 h (evaporation smaller than 0.0004 of the mass). Refractive indexes of each phase were measured and compositions were determined by reference to the curves.

Source and Purity of Materials:

(1) Eastman Kodak Co.; refluxed 24 h with active CaO, distilled, refluxed 4 h with Ca, distilled; n(20 °C,D)=1.396 15, d(25 °C,4 °C)=0.798 11.
(2) Source not specified; dried with Na, recrystallized several times; f.p.=5.48 °C, n(20 °C,D)=1.501 24, d(25 °C,4 °C) =0.873 57.
(3) redistilled.

Estimated Error:

Not reported.

References:

[1] E. R. Washburn, and C. V. Strandskov, J. Phys. Chem. **48**, 241 (1944).

Components:	**Evaluated by:**
(1) 2-Methyl-1-propanol (isobutanol; isobutyl alcohol); $C_4H_{10}O$; [78-83-1] (2) Cyclohexane; C_6H_{12} ; [110-82-7] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1995.09)

7.2. 2-Methyl-1-propanol + Water + Cyclohexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-methyl-1-propanol–cyclohexane–water is given in Table 67.

TABLE 67. Summary of experimental data for the system 2-methyl-1-propanol–cyclohexane–water

Author(s)	T/K	Type of data[a]	Ref.
Plackov and Stern, 1990	298	sat. (14), eq. (7)	1
Letcher *et al.*, 1991	298	sat. (15), eq. (4)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 2-methyl-1-propanol–cyclohexane–water forms a miscibility gap of type 2. The system was studied at 298.2 K by titration method. Two binary systems cyclohexane–water and 2-methyl-1-propanol–water form miscibility gaps. The data of these binary systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. The recommended values of mutual solubility at 298 K are: for the cyclohexane–water system $x_2''=1.2\cdot 10^{-5}$ and $x_3'=3.7\cdot 10^{-4}$,[3] and for the 2-methyl-1-propanol–water system $x_1'=0.548$ and $x_1''=0.0210$.[4] Letcher *et al.*[2] reported ternary data and mutual solubility of the binary systems. The end points of the saturation curve were reported to be $x_2=0.999$ and pure water. This is inconsistent with the recommended values but within the accuracy of the experimental measurements (0.001 mole fraction) stated by the authors. Mutual solubility data for the 2-methyl-1-propanol–water system reported in Ref. 2 as $x_1'=0.546$ and $x_1''=0.021$ are consistent with the ''best values'' reported in the critical evaluation.[3] Plackov and Stern[1] reported the solubility of 2-methyl-1-propanol in water, $x_1''=0.021$. This result is also consistent with recommended data. These experimental data are consistent with one another. Phase equilibrium data were also used to construct the saturation curve of the organic-rich phase. Data at 298.2 K were described by the equation:

$$x_1=0.694\,59+0.031\,38\ \ln(x_2)-0.410\,19x_2-0.293\,07x_2^2.$$

The model describes the region $0.01<x_2<0.99$. The parameters were calculated by the least-squares method. The standard error of estimate was 0.0062. The points on the saturation curve calculated by this equation for selected concentrations of cyclohexane in the mixture are presented in Table 68 and in Fig. 35 as a calculated binodal curve (solid line).

TABLE 68. Calculated compositons along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.548	0.0000 Ref. 4	0.3683	0.5400
0.5635	0.0200	0.3548	0.5600
0.5767	0.0400	0.3410	0.5800
0.5806	0.0600	0.3269	0.6000
0.5806	0.0800	0.3126	0.6200
0.5784	0.1000	0.2980	0.6400
0.5746	0.1200	0.2832	0.6600
0.5697	0.1400	0.2680	0.6800
0.5639	0.1600	0.2527	0.7000
0.5574	0.1800	0.2370	0.7200
0.5503	0.2000	0.2211	0.7400
0.5426	0.2200	0.2050	0.7600
0.5345	0.2400	0.1885	0.7800
0.5259	0.2600	0.1719	0.8000
0.5168	0.2800	0.1550	0.8200
0.5074	0.3000	0.1378	0.8400
0.4976	0.3200	0.1203	0.8600
0.4874	0.3400	0.1027	0.8800
0.4769	0.3600	0.0847	0.9000
0.4660	0.3800	0.0666	0.9200
0.4549	0.4000	0.0481	0.9400
0.4434	0.4200	0.0294	0.9600
0.4316	0.4400	0.0105	0.9800
0.4195	0.4600	0.0010	0.9900
0.4071	0.4800	0.0000	0.999 63 Ref. 3
0.3945	0.5000	0.0000	0.000 012 Ref. 3
0.3815	0.5200	0.0210	0.000 0 Ref. 4

Compositions of the water-rich phase of the ternary system, Refs. 1 and 2, were reported as a binary 2-methyl-1-propanol–water mixture; the analytical methods could not detect cyclohexane. Therefore the water-rich branch could not be evaluated.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 2-methyl-1-propanol–cyclohexane–water were reported in two references at 298.2 K using similar experimental procedures. First the equilibrium was reached, then the phases were separated and the composition of each phase was determinated. Compositions of water-rich phase in equilibrium were reported as binary 2-methyl-1-propanol–water mixture. The analytical methods could not detect cyclohexane. The tie lines cover the whole area of the miscibility gap and are consistent within each data set and with one another with the exception of one experimental tie line of Letcher *et al.*[2] at the lowest 2-methyl-1-propanol concentration ($x_1''=0.007$), which is in disagreement with the corresponding tie line of Plackov and Stern.[1] This could be noticed if a large scale graph were plotted. Both data sets are treated as tentative. All experimental data points at 298.2 K are reported in Fig. 35.

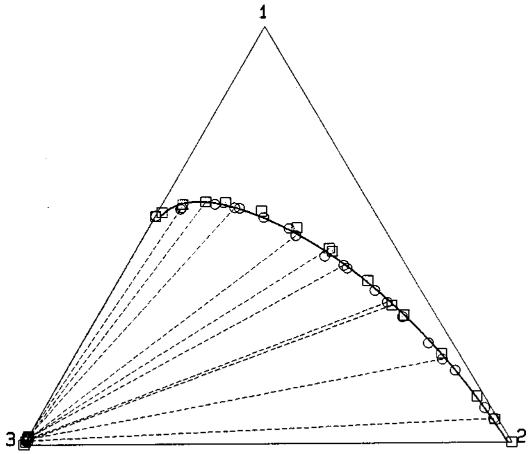

FIG. 35. Phase diagram of the system 2-methyl-1-propanol (1)—cyclohexane (2)—water (3) at 298.2 K. Solid line—calculated binodal curve, ○—experimental results of Ref. 1, □—experimental results of Ref. 2, dashed lines—experimental tie lines, Refs. 1 and 2.

References:

[1] D. Plackov and I. Stern, Fluid Phase Equilib. **57**, 327 (1990).

[2] T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118 (1991).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[4] A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 2-Methyl-1-propanol (isobutanol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. Plackov and I. Stern, Fluid Phase Equilib. **57**, 327–40 (1990).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.00	298.15	0.0825	0.9031	0.0742	0.9226
		0.1721	0.7992	0.1584	0.8352
		0.2384	0.7120	0.2251	0.7635
		0.3017	0.6276	0.2925	0.6908
		0.3654	0.5394	0.3650	0.6118
		0.4192	0.4555	0.4336	0.5349
		0.4484	0.3949	0.4796	0.4796
		0.5156	0.2883	0.5789	0.3676
		0.5426	0.2230	0.6363	0.2969
		0.5648	0.1624	0.6926	0.2261
		0.5748	0.1069	0.7431	0.1569
		0.5667	0.0436	0.7971	0.0696
		0.5470	0.0000	0.8324	0.0000
		0.0207	0.0000	0.0800	0.0000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.00	298.15	0.057	0.934	0.009	0.000	0.051	0.947	0.036	0.000
		0.199	0.760	0.012	0.000	0.186	0.805	0.048	0.000
		0.337	0.579	0.013	0.000	0.332	0.648	0.051	0.000
		0.426	0.445	0.014	0.000	0.442	0.525	0.055	0.000
		0.498	0.311	0.015	0.000	0.555	0.393	0.059	0.000
		0.566	0.152	0.017	0.000	0.701	0.215	0.066	0.000
		0.563	0.043	0.019	0.000	0.796	0.069	0.074	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, as reported in Ref. 1, was used to determine the solubility curve. Mixtures of known composition, mixed by means of a magnetic stirrer and placed in the thermostated double-wall Erlenmayer flask, were titrated with the less soluble component until the appearance of turbidity. The analytical method was used to determine liquid–liquid equilibria. The mixture was shaken for at least 20 min. Equilibration took place in a thermostated double-walled separatory funnel of 250 mL over 2 h. The refractive index and density of both phases were measured. The composition was calculated numerically from the calibration data by polynomial regression analysis. The third order polynomials were used. Each experiment was repeated three times.

Source and Purity of Materials:

(1) Kemoka (Zagreb), analytical grade; used as received; $n = 1.3933$, $\rho(25\ °C) = 794.4$ kg m^{-3}, b.p.=107.9 °C.
(2) Kemika (Zagreb), analytical grade; used as received; $n = 1.4232$, $\rho(25\ °C) = 773.6$ kg m^{-3}, b.p.=80.0 °C.
(3) double distilled in the presence of $KMnO_4$.

Estimated Error:

temp. ±0.02 °C; composition $<\pm 0.05\%$ (by mass) relative error.

References:

[1] E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transuel, J. Am. Chem. Soc. **62**, 1454 (1940).

Components:

(1) 2-Methyl-1-propanol (isobutanol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118–21 (1991).

Variables:

$T/K=298$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$ (compiler)	T/K	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.021	0.000	0.081	0.000
		0.546	0.000	0.832	0.000
		0.555	0.009	0.827	0.015
		0.574	0.042	0.803	0.067
		0.579	0.127	0.729	0.181
		0.558	0.211	0.654	0.281
		0.517	0.304	0.571	0.381
		0.460	0.405	0.483	0.483
		0.389	0.513	0.391	0.585
		0.306	0.629	0.295	0.689
		0.213	0.752	0.198	0.794
		0.110	0.874	0.099	0.897
		0.055	0.937	0.049	0.949
		0.000	0.999	0.0000	0.9998

Compositions of coexisting phases

$t/°C$ (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.546	0.000	0.021	0.000	0.832	0.000	0.081	0.000
		0.580	0.086	0.018	0.000	0.764	0.129	0.070	0.000
		0.467	0.395	0.014	0.000	0.492	0.473	0.055	0.000
		0.330	0.592	0.007	0.000	0.323	0.658	0.028	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the titration method, as described in Ref. 1. The formation of a cloudy mixture was observed visually on shaking after addition of a known mass of the third component; syringes were precisely weighed. Tie line compositions were determined by the refractive index method,[2] and a complementary method using the Karl Fischer titration.[3] Measurements were made at pressure of 94.7 kPa.

Source and Purity of Materials:

(1) Merck; AR grade; dried by addition of anhydrous K_2CO_3, distilled; purity > 99.9 mole % by glc.
(2) BDH; Gold label grade; used as received; purity > 99.9 mole % by glc.
(3) not specified.

Estimated Error:

composition ± 0.005 mole fraction (binodal curve), ±0.01 mole fraction (tie lines).

Reference

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35,** 411 (1943).
[3] T. M. Letcher, P. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 2-Methyl-1-propanol (isobutanol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

$T/K = 298$

Compiled by:

A. Skrzecz

7.3. 2-Methyl-1-propanol + Water + Toluene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.021	0.000	0.081	0.000
		0.546	0.000	0.832	0.000
		0.568	0.031	0.807	0.055
		0.572	0.054	0.784	0.092
		0.568	0.111	0.724	0.176
		0.546	0.186	0.648	0.274
		0.511	0.277	0.563	0.380
		0.462	0.372	0.479	0.479
		0.397	0.479	0.388	0.582
		0.315	0.593	0.293	0.686
		0.214	0.722	0.190	0.796
		0.117	0.849	0.099	0.894
		0.060	0.924	0.049	0.947

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.171	0.783	0.005	0.000	0.148	0.842	0.020	0.000
		0.426	0.432	0.011	0.000	0.427	0.538	0.044	0.000
		0.550	0.181	0.017	0.000	0.654	0.268	0.066	0.000
		0.546	0.000	0.021	0.000	0.832	0.000	0.081	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by the addition of anhydrous potassium carbonate, distilled; purity better than 99.6 mole % by glc.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 2-Methyl-1-propanol (isobutanol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]
(2) 1-Heptene; C_7H_{14}; [592-76-7]
(3) Water; H_2O, [7732-18-5]

Original Measurements:

T. M. Letcher, B. C. Bricknell, J. D. Sewry, and S. E. Radloff, J. Chem. Eng. Data **39**, 320–3 (1994).

Variables:

T/K=298

Compiled by:

A. Skrzecz

7.4. 2-Methyl-1-propanol + Water + 1-Heptene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	1.000	0.000	1.000
		0.134	0.848	0.106	0.890
		0.235	0.725	0.195	0.797
		0.365	0.565	0.323	0.662
		0.450	0.440	0.425	0.550
		0.492	0.372	0.483	0.484
		0.519	0.326	0.525	0.437
		0.540	0.285	0.562	0.393
		0.560	0.239	0.605	0.342
		0.576	0.201	0.643	0.297
		0.587	0.162	0.680	0.249
		0.596	0.121	0.722	0.194
		0.599	0.106	0.738	0.173
		0.594	0.071	0.772	0.122
		0.584	0.043	0.798	0.078
		0.548	0.000	0.833	0.000
		0.021	0.000	0.081	0.000
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.595	0.111	0.018	0.000	0.731	0.181	0.070	0.000
		0.549	0.271	0.015	0.000	0.577	0.377	0.059	0.000
		0.424	0.480	0.010	0.000	0.391	0.587	0.040	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods have been described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) Aldrich; distilled; purity >99.8 mole % by glc, $\rho = 0.692\ 65\ \mathrm{g\,cm}^{-3}$.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) 2-Methyl-1-propanol (isobutanol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]
(2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053–60 (1989).

Variables:

T/K=298

Compiled by:

A. Skrzecz

7.5. 2-Methyl-1-propanol + Water + *p*-Xylene

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.998	0.000	0.9997
		0.069	0.916	0.050	0.948
		0.135	0.843	0.100	0.896
		0.249	0.695	0.198	0.791
		0.345	0.561	0.295	0.686
		0.422	0.444	0.387	0.583
		0.530	0.247	0.565	0.377
		0.558	0.167	0.646	0.277
		0.571	0.105	0.714	0.188
		0.572	0.011	0.830	0.023
		0.548	0.000	0.833	0.000
		0.021	0.000	0.081	0.000

Compositions of coexisting phases

t/°C (compiler)	T/K	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.548	0.000	0.021	0.000	0.833	0.000	0.081	0.000
		0.510	0.282	0.014	0.000	0.529	0.419	0.055	0.000
		0.257	0.685	0.008	0.000	0.205	0.784	0.032	0.000
		0.000	0.998	0.000	0.000	0.000	0.9997	0.000	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. A binary mixture of known composition was titrated with the third component until cloudiness was observed. Tie line compositions were related to the coexistence curve; water was determined by the Karl Fischer titration. The methods were described in Ref. 1.

Source and Purity of Materials:

(1) source not specified; used as received.
(2) source not specified; recrystallized three times.
(3) not specified.

Estimated Error:

comp. <0.005 mole fraction (estimated authors' precision on binodal curve), <0.01 mole fraction (estimated authors' precision of tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

Components:

(1) 2-Methyl-1-propanol (isobutanol, isobutyl alcohol); $C_4H_{10}O$; [78-83-1]
(2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12}; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

7.6. 2-Methyl-1-propanol + Water + Mesitylene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.021	0.000	0.081	0.000
		0.546	0.000	0.832	0.000
		0.560	0.021	0.805	0.049
		0.577	0.089	0.719	0.180
		0.568	0.150	0.646	0.276
		0.549	0.226	0.566	0.378
		0.504	0.311	0.479	0.479
		0.445	0.413	0.387	0.583
		0.368	0.531	0.294	0.687
		0.271	0.670	0.198	0.792
		0.149	0.825	0.100	0.896
		0.077	0.906	0.050	0.948
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.205	0.752	0.007	0.000	0.143	0.850	0.028	0.000
		0.382	0.509	0.011	0.000	0.310	0.669	0.044	0.000
		0.503	0.312	0.016	0.000	0.477	0.480	0.063	0.000
		0.546	0.000	0.021	0.000	0.832	0.000	0.081	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by the addition of anhydrous potassium carbonate, distilled; purity better than 99.6 mole % by glc.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:[1]T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2]S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3]T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radolff, J. Chem. Thermodyn. **21**, 1053 (1989).

8. 2-Methyl-2-propanol+Water

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) 1-Butene; C_4H_8; [106-98-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

I. I. Vasileva, A. A. Naymova, A. A. Polyakov, T. N. Tyvina, V. V. Fokina, and N. G. Khrabrova, Zh. Prikl. Khim. (Leningrad) **63**, 1432-6 1990. [Eng. transl. Russ. J. Appl. Chem. (Leningrad) **63**, 589–95 (1990)].

Variables:

T/K=293−453

Compiled by:

A. Skrzecz

8.1. 2-Methyl-2-propanol + Water + 1-Butene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
48.0	321.15	0.0582	0.0012	0.2023	0.0032
174.6	447.75	0.0944	0.0057	0.2974	0.0136
137.8	410.95	0.1030	0.0039	0.3189	0.0091
10.0	283.15	0.1034	0.0039	0.3198	0.0091
180.8	453.95	0.1156	0.0110	0.3438	0.0248
126.2	399.35	0.1161	0.0053	0.3480	0.0120
136.4	409.55	0.1399	0.0070	0.3968	0.0150
39.0	312.15	0.1399	0.0073	0.3967	0.0157
182.0	455.15	0.1652	0.0231	0.4348	0.0460
133.8	406.95	0.1662	0.0109	0.4438	0.0220
40.5	313.65	0.1664	0.0114	0.4439	0.0230
138.6	411.75	0.2155	0.0172	0.5193	0.0314
79.9	353.05	0.2542	0.0237	0.5679	0.0401
107.0	380.15	0.2542	0.0237	0.5679	0.0401
129.2	402.35	0.3220	0.0564	0.6243	0.0828
118.0	391.15	0.3271	0.0542	0.6309	0.0791
57.0	330.15	0.3271	0.0542	0.6309	0.0791
100.0	373.15	0.3559	0.0735	0.6468	0.1011
135.6	408.75	0.3875	0.1167	0.6498	0.1481
105.0	378.15	0.4374	0.3487	0.5806	0.3504
143.0	416.15	0.3780	0.4415	0.5000	0.4420
180.0	453.15	0.3152	0.4680	0.4365	0.4906

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''	
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		p/kPa
20	293.2	0.000 00	0.999 906	0.000 00	0.000 23	0.000 00	0.999 97	0.000 00	0.000 72	
		0.000 70	0.998 10	0.002 90	0.000 23	0.000 93	0.998 69	0.011 82	0.000 71	
		0.0204	0.9774	0.010 80	0.000 27	0.0268	0.9725	0.042 97	0.000 81	
		0.0347	0.9624	0.016 00	0.000 27	0.0454	0.9536	0.062 67	0.000 80	
		0.1389	0.0070	0.1389	0.0070	0.3948	0.0151	0.3948	0.0151[a]	
40	313.2	0.1389	0.0070	0.1389	0.0070	0.3948	0.0151	0.3948	0.0151[a]	
80	353.2	0.0000	0.9916	0.0000	0.000 27	0.0000	0.9973	0.000 00	0.000 84	1200
		0.0149	0.9753	0.0019	0.000 27	0.0197	0.9771	0.007 77	0.000 84	1160
		0.0615	0.9123	0.0068	0.000 30	0.0811	0.9105	0.027 38	0.000 91	1080
		0.3384	0.0709	0.0452	0.000 73	0.6318	0.1002	0.162 80	0.001 99	690
		0.1389	0.0070	0.1389	0.0070	0.3948	0.0151	0.3948	0.0151	390[a]
138	411.2	0.0000	0.9575	0.000 00	0.000 58	0.0000	0.9859	0.000 00	0.001 80	3790
		0.1068	0.8255	0.003 90	0.000 58	0.1428	0.8352	0.015 83	0.001 78	3230
		0.4102	0.3232	0.015 80	0.007 60	0.5700	0.3400	0.061 02	0.022 22	2450
		0.3323	0.0584	0.042 50	0.001 09	0.6334	0.0843	0.154 11	0.002 99	1530
		0.1389	0.0070	0.1389	0.0070	0.3948	0.0151	0.3948	0.0151	1000[a]
154	427.2	0.1396	0.0093	0.1396	0.0093	0.3949	0.0199	0.3949	0.0199	1840[a]
180	453.2	0.1384	0.0141	0.1384	0.0141	0.3898	0.0301	0.3898	0.0301	2500[a]

[a] Plait point.

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method with glass ampoules, described in Ref. 1, was used to visually determine the phase transition (mass of components in the vapor phase was neglected). Temperature was measured with a mercury thermometer. Compositions of coexisting phases in equilibrium (two liquids and vapor) were determined in a static apparatus. The liquid phases were analyzed by glc. (The pressure was reported during the measurements at temperatures higher than 353.2 K).

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

temp. ±0.2 °C (saturation curve) and ±0.5 °C (phase equilibrium).

References:

[1] C. M. Khodeeva, and E. C. Lebedeva, Zh. Fiz. Khim. **40,** 3105 (1966).

Components:	**Evaluated by:**
(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0] (2) Benzene; C_6H_6 ; [71-43-2] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.05)

8.2. 2-Methyl-2-propanol + Water + Benzene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-methyl-2-propanol–benzene–water is given in Table 69.

TABLE 69. Summary of experimental data for the system 2-methyl-2-propanol–benzene–water

Author(s)	T/K	Type of data[a]	Ref.
Simonsen and Washburn, 1946	298	sat. (34), eq. (11)	1
Letcher *et al.*, 1990	298	sat. (13), eq. (4)	2

[a] Number of experimental points in parentheses.

The ternary system 2-methyl-2-propanol–benzene–water forms a miscibility gap of type 1. Only one binary system benzene–water forms a miscibility gap. These binary data were compiled and critically evaluated in a previously published SDS volume, Ref. 3. The recommended values of mutual solubility at 298 K are $x_2'=0.9970$, $x_2''=0.000\ 409$. The mutual solubility of benzene and water was also reported by Simonsen and Washburn, [1] ($x_2'=0.9970$, $x_2''=0.0003$); these are consistent with the recommended values. Letcher *et al.* [2] reported data only in graphical form. Therefore these data are not compiled. The plait point estimated by Letcher and Siswana[4] was $x_1=0.16$ and $x_2=0.02$, while the maximum alcohol concentration on the binodal curve is $x_1=0.41$. This point is consistent with the results of Simonsen and Washburn measurements, $x_1=0.38$.[1] The experimental tie lines at 298.2 K[1] are presented in Fig. 36 together with the experimental points along the saturation curve.

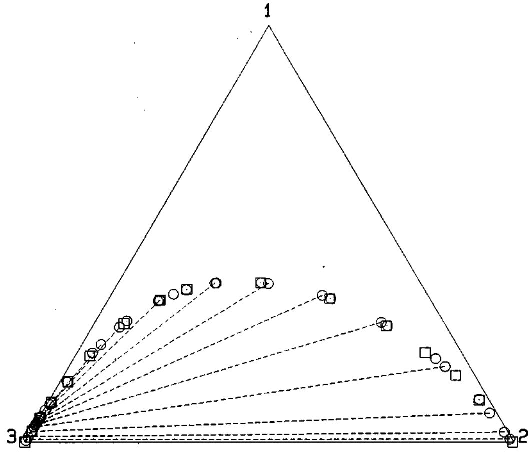

FIG. 36. Phase diagram of the system 2-methyl-2-propanol (1)—benzene (2)—water (3) at 293.2 K. ○—experimental results, Ref. 1, set 1, □—experimental results, Ref. 1, set 2, dashed lines—experimental tie lines, Ref. 1.

References:

[1] D. R. Simonsen and E. R. Washburn, J. Am. Chem. Soc. **68**, 235 (1946).

[2] T. M. Letcher, J. Sewry, and S. Radloff, S. Afr. J. Chem. **43**, 56 (1990).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[4] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. R. Simonsen and E. R. Washburn, J. Am. Chem. Soc. **68**, 235–7 (1946).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2	
		(compiler)				
25.0	298.15	0.1022	0.8779	0.0990	0.8963	(series I)
		0.1991	0.7404	0.2003	0.7849	
		0.2776	0.6027	0.2947	0.6744	
		0.3433	0.4542	0.3941	0.5494	
		0.3814	0.2925	0.4960	0.4009	
		0.3802	0.2008	0.5481	0.3051	
		0.3642	0.1470	0.5709	0.2429	
		0.3534	0.1260	0.5768	0.2167	
		0.3369	0.1029	0.5794	0.1865	
		0.2894	0.0629	0.5640	0.1292	
		0.2131	0.0311	0.4961	0.0762	
		0.1442	0.0140	0.3967	0.0406	
		0.0950	0.0056	0.2974	0.0184	
		0.0576	0.0014	0.2001	0.0052	
		0.0413	0.0011	0.1501	0.0041	
		0.0260	0.0007	0.0988	0.0027	
25.0	298.15	0.0000	0.9970	0.0000	0.9993	(series II)
		0.1006	0.8781	0.0976	0.8974	
		0.1595	0.8009	0.1574	0.8331	
		0.2137	0.7115	0.2177	0.7638	
		0.2771	0.6010	0.2948	0.6737	
		0.3430	0.4524	0.3945	0.5483	
		0.3814	0.2915	0.4965	0.4000	
		0.3651	0.1475	0.5714	0.2432	
		0.3393	0.1055	0.5795	0.1900	
		0.2832	0.0594	0.5602	0.1238	
		0.2058	0.0290	0.4873	0.0724	
		0.1450	0.0147	0.3976	0.0424	
		0.0962	0.0058	0.3002	0.0190	
		0.0584	0.0014	0.2024	0.0051	
		0.0268	0.0007	0.1014	0.0026	
		0.0000	0.0003	0.0000	0.0015	

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_1''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.15	0.0068	0.9876	0.0040	0.0004	0.0065	0.9922	0.0162	0.0017
		0.0234	0.9680	0.0124	0.0005	0.0224	0.9756	0.0490	0.0022
		0.0695	0.9151	0.0247	0.0007	0.0670	0.9294	0.0940	0.0027
		0.1803	0.7689	0.0357	0.0008	0.1798	0.8079	0.1317	0.0033
		0.2854	0.5865	0.0415	0.0010	0.3054	0.6613	0.1508	0.0038
		0.3504	0.4334	0.0455	0.0011	0.4076	0.5313	0.1636	0.0040
		0.3793	0.3086	0.0490	0.0011	0.4861	0.4167	0.1744	0.0043
		0.3799	0.1979	0.0528	0.0013	0.5497	0.3018	0.1858	0.0047
		0.3388	0.1053	0.0618	0.0017	0.5793	0.1897	0.2123	0.0060
		0.2742	0.0551	0.0767	0.0031	0.5537	0.1172	0.2526	0.0108
		0.2332	0.0379	0.0905	0.0049	0.5178	0.0888	0.2867	0.0164

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine the solubility curve. Binary mixtures were titrated until the second phase appeared in 50 mL flasks with mechanical shaker placed in thermostated bath. Very small drops (5 mg of water and 4 mg of benzene) were added from capillary-tipped pipettes. An hour of shaking, after the last drop, was sufficient for complete saturation. Two independent series were made. In the series I, refractive indexes were measured by Abbe refractometer; in the series II, specific gravities were measured by glass-stoppered, capillary steamed 5 mL pycnometers and viscosities were measured by ordinary Ostwald viscometers. Conjugate solutions were prepared by adding calculated amounts of each component successively to 25 mL glass-stoppered flasks. Shaking in a constant temperature bath was continued until constant refractive indexes of both phases were observed. After 1/2 h separation the final refractive indexes of both phases were measured and the compositions were determined from the previously prepared graphs. The method was similar to that described in Refs. 1, 2, 3.

Source and Purity of Materials:

(1) Eastman Kodak Company, recrystallized several times; $d(25\ °C,4\ °C)=0.780\ 43$, $n(25\ °C,D)=1.384\ 83$, f.p. $=25.66$ °C.
(2) Coleman and Bell, reagent quality grade, dried with Na and slowly distilled; middle fraction was recrystallized several times; $d(25\ °C,4\ °C)=0.780\ 43$, $n(25\ °C,D)=1.384\ 83$, f.p. $=25.66$ °C.
(3) redistilled

Estimated Error:

temp. ±0.04 °C (temperature of the bath).

References:

[1] E. R. Washburn, V. Hnizda, and R. Vold, J. Am. Chem. Soc. **53**, 3237 (1931).
[2] E. R. Washburn and C. V. Strandskov, J. Phys. Chem. **48**, 241 (1944).
[3] Alberty and E. R. Washburn, J. Phys. Chem. **49**, 4 (1945).

Components:	**Evaluated by:**
(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0] (2) Cyclohexane; C_6H_{12} ; [110-82-7] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, (1997.03)

8.3. 2-Methyl-2-propanol + Water + Cyclohexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-methyl-2-propanol–cyclohexane–water is given in Table 70.

TABLE 70. Summary of experimental data for the system 2-methyl-2-propanol–cyclohexane–water

Author(s)	T/K	Type of data[a]	Ref.
Plackov and Stem, 1990	298	sat. (19), eq. (7)	1
Letcher *et al.*, 1991	298	sat. (15), eq. (5)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 2-methyl-2-propanol–cyclohexane–water forms a miscibility gap of type 1. The system was investigated twice at 298 K by titration method. Only the binary system cyclohexane–water forms a miscibility gap. Data of this system were compiled and critically evaluated in a previously published SDS volume,[3] the recommended values at 298 K are: $x_2''=1.2\cdot 10^{-5}$ and $x_3'=3.7\cdot 10^{-4}$. The saturated binary cyclohexane–water mixtures reported in Ref. 2 as $x_2''=0.0$ and $x_3'=0.001$ are the result of the limited analytical methods used. The systems 2-methyl-2-propanol–water and 2-methyl-2-propanol–cyclohexane are miscible. The saturation data[1,2] are consistent with one another and with the recommended values for the binary system. All experimental solubility and equilibrium data reported in Refs. 1 and 2 were used for calculation of saturation curve. These data were described by the equation:

$$x_1=a_1\cdot(-\ln z_1)^{a_2}\cdot z_1{}^{d_3},$$

where: $z_1=(x_2+0.5\cdot x_1-x_{20}'')/(x_{20}'-x_{20}'')$, x_1, x_2—mole fractions of component (1) and (2), respectively, x_{20}', x_{20}''—values of x_2 on the binodal curve which cuts the $x_1=0$ axis.

This equation has been proposed by Letcher *et al.*[4] for the description of saturation curves of ternary alcohol–ether–water systems. It gives better results (the smallest standard deviation) for the investigated system than any other tested equation. The parameters obtained by the least-squares method for the whole range of miscibility gap (water-rich and hydrocarbon-rich branches were described together) are: $a_1=1.469\ 36$, $a_2=0.972\ 29$, $a_3=1.277\ 11$. The standard error of estimate was 0.0044. For selected concentrations of cyclohexane in the mixture the saturation curve was calculated. The results are presented in Table 71 and in Fig. 37 as solid line.

TABLE 71. Calculated compositons along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.0000	0.000 012 Ref. 3	0.3465	0.5200
0.1574	0.0100	0.3360	0.5400
0.2112	0.0200	0.3251	0.5600
0.2753	0.0400	0.3137	0.5800
0.3165	0.0600	0.3020	0.6000
0.3462	0.0800	0.2898	0.6200
0.3685	0.1000	0.2773	0.6400
0.3855	0.1200	0.2644	0.6600
0.3986	0.1400	0.2512	0.6800
0.4085	0.1600	0.2376	0.7000
0.4158	0.1800	0.2237	0.7200
0.4210	0.2000	0.2096	0.7400
0.4243	0.2200	0.1951	0.7600
0.4260	0.2400	0.1803	0.7800
0.4262	0.2600	0.1653	0.8000
0.4252	0.2800	0.1500	0.8200
0.4230	0.3000	0.1344	0.8400
0.4199	0.3200	0.1185	0.8600
0.4158	0.3400	0.1024	0.8800
0.4108	0.3600	0.0860	0.9000
0.4050	0.3800	0.0694	0.9200
0.3985	0.4000	0.0525	0.9400
0.3913	0.4200	0.0353	0.9600
0.3834	0.4400	0.0178	0.9800
0.3750	0.4600	0.0089	0.9900
0.3660	0.4800	0.0000	0.999 63 Ref. 3
0.3565	0.5000		

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the 2-methyl-2-propanol–cyclohexane–water system were reported in both references and similar experimental procedures were used. In the first step the equilibrium was reached and then the phases were separated and the composition of each phase was analyzed. Compositions of water-rich phase of the ternary system in both references show very low concentration of cyclohexane (0–0.001 and 0.003–0.007 mole fraction in Refs. 1 and 2, respectively). The tie lines cover the whole area of the miscibility gap. They are consistent within each data set. Data of Plackov and Stern[1] cover the area of the lower concentrations of cyclohexane while the data of Letcher *et al.*[2] cover the area of the higher concentrations of hydrocarbon. The areas overlap slightly with one another; their directions differ a little. Letcher *et al.*[2] report lower concentrations of alcohol in water-rich phase than Plackov and Stern;[1] consequently the tie lines cross. Both data sets are treated as tentative. All experimental points at 298.2 K, both saturation and for phases in equilibrium, Refs. 1 and 2, are presented in Fig. 37.

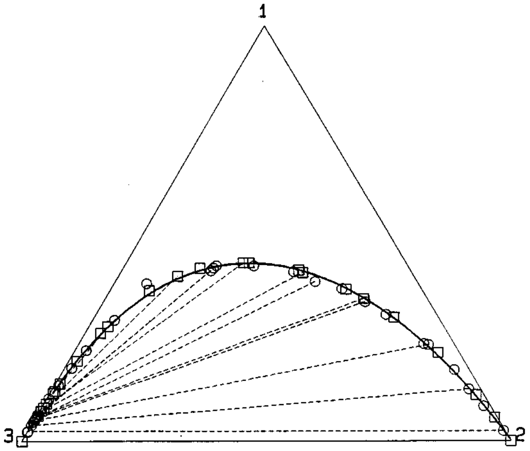

FIG. 37. Phase diagram of the system 2-methyl-2-propanol (1)—cyclohexane (2)—water (3) at 298.2 K. Solid line—calculated binodal curve, ○—experimental results, Ref. 1, □—experimental results, Ref. 2, dashed lines—experimental tie lines, Refs. 1 and 2.

References:

[1] D. Plackov and I. Stern, Fluid Phase Equilib. **57**, 327 (1990).
[2] T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118 (1991).
[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).
[4] T. M. Letcher, S. Ravindran, and S. E. Radloff, Fluid Phase Equilib. **69**, 251 (1991).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. Plackov and I. Stern, Fluid Phase Equilib. **57**, 327–40 (1990).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
25.00	298.15	0.0832	0.9018	0.0749	0.9218
		0.1702	0.7982	0.1570	0.8359
		0.2321	0.7045	0.2224	0.7631
		0.3036	0.5923	0.3032	0.6716
		0.3658	0.4723	0.3886	0.5696
		0.4071	0.3537	0.4696	0.4633
		0.4217	0.2654	0.5277	0.3771
		0.4164	0.1850	0.5757	0.2904
		0.3783	0.0658	0.6432	0.1270
		0.2903	0.0439	0.5783	0.0993
		0.2178	0.0224	0.5090	0.0594
		0.1753	0.0142	0.4513	0.0415
		0.1342	0.0076	0.3819	0.0246
		0.1027	0.0035	0.3171	0.0123
		0.0731	0.0010	0.2443	0.0038
		0.0599	0.0004	0.2074	0.0016
		0.0510	0.0003	0.1809	0.0012
		0.0455	0.0002	0.1639	0.0008
		0.0216	0.0002	0.0832	0.0009

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.00	298.15	0.024	0.972	0.024	0.000	0.021	0.978	0.092	0.000
		0.124	0.851	0.038	0.000	0.113	0.881	0.140	0.000
		0.231	0.715	0.047	0.001	0.219	0.769	0.168	0.004
		0.334	0.535	0.053	0.001	0.343	0.624	0.187	0.004
		0.383	0.409	0.055	0.001	0.426	0.517	0.193	0.004
		0.422	0.188	0.059	0.001	0.578	0.292	0.204	0.004
		0.410	0.183	0.064	0.001	0.572	0.290	0.219	0.004

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, as reported in Ref. 1, was used to determine the solubility curve. Mixtures of known composition, mixed by means of a magnetic stirrer and placed in the thermostated double-wall Erlenmayer flask, were titrated with the less soluble component until the appearance of turbidity. The analytical method was used to determine liquid–liquid equilibria. The mixture was shaken for at least 20 min. Equilibration took place in a thermostated double-walled separatory funnel of 250 mL over 2 h. The refractive index and density of both phases were measured. The composition was calculated numerically from the calibration data by polynomial regression analysis. The third order polynomials were used. Each experiment was repeated three times.

Source and Purity of Materials:

(1) Merck, analytical grade; used as received; $n=1.3847$, b.p. $=99.3$ °C.
(2) Kemika (Zagreb), analytical grade; used as received; $n=1.4232$, $\rho(25\ °C)=773.6$ kg m^{-3}, b.p.$=80.0$ °C.
(3) double distilled in the presence of $KMnO_4$.

Estimated Error:

temp. ±0.02 °C; composition <± 0.05% (by mass) relative error.

References:

[1] E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transuel, J. Am. Chem. Soc. **62**, 1454 (1940).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118–21 (1991).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.115	0.006	0.343	0.020
		0.138	0.009	0.388	0.029
		0.192	0.017	0.476	0.048
		0.259	0.031	0.555	0.075
		0.361	0.080	0.614	0.155
		0.416	0.157	0.596	0.255
		0.429	0.252	0.541	0.361
		0.411	0.362	0.469	0.469
		0.364	0.481	0.384	0.576
		0.297	0.612	0.293	0.685
		0.212	0.744	0.199	0.791
		0.110	0.873	0.100	0.897
		0.056	0.938	0.050	0.949
		0.000	0.999	0.0000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.342	0.528	0.060	0.003	0.351	0.616	0.206	0.012
		0.405	0.373	0.072	0.003	0.459	0.480	0.240	0.011
		0.429	0.240	0.080	0.004	0.549	0.348	0.260	0.015
		0.396	0.121	0.090	0.005	0.609	0.211	0.285	0.018
		0.275	0.038	0.120	0.007	0.567	0.089	0.353	0.023

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the titration method, as described in Ref. 1. The formation of a cloudy mixture was observed visually on shaking after addition of a known mass of the third component; syringes were precisely weighed. Tie line compositions were determined by the refractive index method, Ref. 2, and a complementary method using the Karl Fischer titration, Ref. 3. Measurements were made at pressure of 94.7 kPa.

Source and Purity of Materials:

(1) Merck; AR grade; dried by addition of anhydrous K_2CO_3, distilled; purity >99.9 mole % by glc.
(2) BDH; Gold label grade; used as received; purity >99.9 mole % by glc.
(3) not specified.

Estimated Error:

composition ±0.005 mole fraction (binodal curve), ±0.01 mole fraction (tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:	**Original Measurements:**
(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0] (2) Toluene (methylbenzene); C_7H_8; [108-88-3] (3) Water; H_2O; [7732-18-5]	T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).
Variables: T/K=298	**Compiled by:** A. Skrzecz

8.4. 2-Methyl-2-propanol + Water + Toluene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.057	0.002	0.198	0.009
		0.138	0.010	0.386	0.035
		0.191	0.021	0.467	0.064
		0.257	0.038	0.540	0.099
		0.307	0.062	0.571	0.143
		0.375	0.129	0.572	0.244
		0.411	0.205	0.541	0.336
		0.391	0.319	0.456	0.462
		0.363	0.438	0.380	0.570
		0.305	0.573	0.291	0.680
		0.220	0.707	0.197	0.787
		0.116	0.855	0.098	0.896
		0.060	0.928	0.049	0.948

Compositions of coexisting phase

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.140	0.835	0.025	0.001	0.118	0.877	0.095	0.005
		0.256	0.653	0.040	0.002	0.235	0.745	0.145	0.009
		0.361	0.416	0.058	0.003	0.387	0.555	0.200	0.013
		0.398	0.203	0.077	0.004	0.533	0.338	0.252	0.016
		0.372	0.127	0.090	0.006	0.571	0.242	0.284	0.024
		0.298	0.060	0.114	0.009	0.564	0.141	0.337	0.033

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by the addition of anhydrous potassium carbonate, distilled; purity better than 99.6 mole % by glc.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) 1-Heptene; C_7H_{14}; [592-76-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, B. C. Bricknell, J. D. Sewry, and S. E. Radloff, J. Chem. Eng. Data **39**, 320–3 (1994).

Variables:

T/K=298

Compiled by:

A. Skrzecz

8.5. 2-Methyl-2-propanol + Water + 1-Heptene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	1.000	0.000	1.000
		0.151	0.820	0.121	0.873
		0.255	0.688	0.216	0.772
		0.346	0.563	0.311	0.670
		0.403	0.421	0.402	0.556
		0.437	0.283	0.497	0.426
		0.430	0.200	0.548	0.338
		0.401	0.122	0.591	0.238
		0.345	0.061	0.605	0.142
		0.299	0.040	0.583	0.103
		0.219	0.021	0.507	0.064
		0.189	0.012	0.474	0.040
		0.152	0.009	0.413	0.032
		0.109	0.003	0.332	0.012
		0.079	0.001	0.260	0.004
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.275	0.033	0.032	0.001	0.565	0.090	0.119	0.005
		0.355	0.070	0.045	0.001	0.604	0.158	0.162	0.005
		0.398	0.116	0.055	0.002	0.594	0.229	0.192	0.009
		0.437	0.241	0.074	0.003	0.524	0.383	0.245	0.013
		0.409	0.422	0.105	0.004	0.405	0.554	0.321	0.016
		0.345	0.565	0.135	0.005	0.309	0.671	0.385	0.019

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods have been described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) Aldrich; distilled; purity>99.8 mole% by glc, $\rho=0.692\,65$ g cm^{-3}.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:

T/K=298

Compiled by:

A. Skrzecz

8.6. 2-Methyl-2-propanol + Water + Heptane

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.072	0.000	0.242	0.000
		0.154	0.006	0.420	0.022
		0.191	0.014	0.474	0.047
		0.330	0.055	0.596	0.134
		0.404	0.120	0.592	0.238
		0.432	0.295	0.482	0.445
		0.342	0.557	0.305	0.673
		0.267	0.683	0.222	0.768
		0.078	0.911	0.059	0.939

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C (compiler)	T/K	hydrocarbon-rich phase		water -rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.427	0.160	0.090	0.000	0.574	0.291	0.289	0.000
		0.423	0.351	0.054	0.000	0.444	0.498	0.190	0.000
		0.212	0.762	0.019	0.000	0.170	0.825	0.074	0.000
		0.127	0.863	0.009	0.000	0.098	0.900	0.036	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) Aldrich, Gold label, 99.5 mole %; dried with anhydrous potassium carbonate, filtrated, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1] S. W. Briggs and E. W. Commings, Ind. Eng. Chem. **35**, 411 (1943).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn, **21**, 1053–60 (1989).

Variables:

T/K=298

Compiled by:

A. Skrzecz

8.7. 2-Methyl-2-propanol + Water +*p*-Xylene

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.998	0.000	0.9997
		0.070	0.915	0.051	0.947
		0.133	0.837	0.099	0.895
		0.243	0.680	0.197	0.788
		0.327	0.533	0.291	0.679
		0.385	0.403	0.380	0.569
		0.412	0.287	0.460	0.459
		0.411	0.191	0.526	0.350
		0.369	0.111	0.564	0.243
		0.310	0.054	0.572	0.143
		0.224	0.023	0.509	0.075
		0.164	0.012	0.430	0.045
		0.115	0.005	0.342	0.021
		0.041	0.003	0.148	0.015
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C (compiler)	T/K	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.246	0.030	0.123	0.009	0.529	0.092	0.355	0.037
		0.382	0.131	0.055	0.002	0.555	0.273	0.192	0.010
		0.409	0.305	0.030	0.001	0.447	0.477	0.112	0.005
		0.367	0.444	0.018	0.001	0.350	0.606	0.070	0.006
		0.332	0.522	0.015	0.000	0.298	0.670	0.059	0.000
		0.212	0.723	0.005	0.000	0.168	0.820	0.020	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. A binary mixture of known composition was titrated with the third component until cloudiness was observed. Tie line compositions were related to the coexistence curve; water was determined by the Karl Fischer titration. The methods were described in Ref. 1.

Source and Purity of Materials:

(1) source not specified; used as received.
(2) source not specified; recrystallized three times.
(3) not specified.

Estimated Error:

comp. <0.005 mole fraction (estimated authors' precision on binodal curve), <0.01 mole fraction (estimated authors' precision of tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) 2,4,4-Trimethylpentene (diisobutylene isomer not specified); C_8H_{16}; [25167-70-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Y. Y. Lee, Y.-W. Lee, W.-H. Hong, and H. Lee, J. Chem. Eng. Data **33**, 258–60 (1988).

Variables:

T/K=298–348

Compiled by:

A. Skrzecz

8.8. 2-Methyl-2-propanol + Water + 2,4,4-Trimethylpentene

Experimental Data

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.0387	0.9601	0.0192	0.0001	0.0259	0.9739	0.0745	0.0006
		0.1208	0.8762	0.0267	0.0002	0.0834	0.9161	0.1013	0.0011
		0.2003	0.7372	0.0359	0.0003	0.1504	0.8382	0.1327	0.0017
		0.2953	0.6267	0.0416	0.0003	0.2338	0.7512	0.1513	0.0017
		0.3817	0.4700	0.0462	0.0003	0.3380	0.6301	0.1659	0.0016
		0.4155	0.3617	0.0507	0.0003	0.4085	0.5383	0.1799	0.0016
		0.4313	0.2478	0.0550	0.0003	0.4877	0.4242	0.1929	0.0016
		0.4108	0.1374	0.0590	0.0004	0.5638	0.2855	0.2047	0.0021
		0.3474	0.0702	0.0718	0.0007	0.5836	0.1785	0.2407	0.0036
		0.1132	0.0028	0.1132	0.0028	0.3407	0.0128	0.3407	0.0128[a]
45.0	318.2	0.0525	0.9212	0.0154	0.0001	0.0361	0.9595	0.0604	0.0006
		0.1412	0.8321	0.0230	0.0001	0.1003	0.8951	0.0883	0.0006
		0.2361	0.7058	0.0279	0.0001	0.1790	0.8103	0.1056	0.0006
		0.3318	0.5555	0.0321	0.0001	0.2765	0.7007	0.1200	0.0006
		0.3888	0.4504	0.0354	0.0002	0.3504	0.6144	0.1311	0.0011
		0.4309	0.3314	0.0396	0.0001	0.4351	0.5066	0.1450	0.0006
		0.4367	0.2243	0.0427	0.0002	0.5086	0.3955	0.1549	0.0011
		0.4164	0.1365	0.0470	0.0002	0.5691	0.2824	0.1685	0.0011
		0.3587	0.0657	0.0550	0.0004	0.5998	0.1663	0.1929	0.0021
		0.0984	0.0016	0.0984	0.0016	0.3079	0.0076	0.3079	0.0076[a]
75.0	348.2	0.0856	0.9030	0.0099	0.0004	0.0588	0.9393	0.0394	0.0024
		0.1705	0.7806	0.0167	0.0001	0.1250	0.8663	0.0653	0.0006
		0.2641	0.6683	0.0205	0.0001	0.2044	0.7829	0.0792	0.0006
		0.3438	0.5375	0.0252	0.0002	0.2898	0.6859	0.0960	0.0012
		0.4112	0.4282	0.0272	0.0002	0.3743	0.5901	0.1031	0.0011
		0.4433	0.3105	0.0295	0.0002	0.4555	0.4830	0.1111	0.0011
		0.4578	0.2155	0.0326	0.0002	0.5302	0.3778	0.1217	0.0011
		0.4407	0.1342	0.0368	0.0002	0.5898	0.2719	0.1357	0.0011
		0.3834	0.0662	0.0415	0.0002	0.6210	0.1623	0.1511	0.0011
		0.0762	0.0009	0.0762	0.0009	0.2524	0.0045	0.2524	0.0045[a]

[a] Plait points estimated by the authors.

Auxiliary Information

Method/Apparatus/Procedure:

The tubes, of 1.5 cm internal diameter and 16 cm long, containing about 20 cm^2 liquid, were placed in a thermostated bath. After 2 h of shaking, mixtures were allowed to separate for 5 h. Samples of each phase were analyzed by glc (Propak-Q, 250 °C, He 50 mL/min) equipped with a thermal conductivity detector connected with integration unit. (Syringes were heated to prevent phase separation.) Mean of four analyzes was reported. Plait points were estimated by the Treybal's method.[1]

Source and Purity of Materials:

(1) Junsei Chem. Co., Ltd., guaranteed reagent grade, certified purity >99.5 mole %; used as received; purity >99.9% by glc.
(2) Wako Pure Chem. Ind. Ltd., guaranteed reagent grade, certified purity >99.5 mole %; used as received; purity >99.9% by glc.
(3) de-ionized, distilled.

Estimated Error:

temp. ±0.2 °C (accuracy of bath control); conc. ±0.0005 mole fraction.

References:

[1] R. E. Treybal, L. D. Weber, and J. F. Daley, Ind. Eng. Chem. **38**, 817 (1946).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) 2,2,4-Trimethylpentane (isooctane); C_8H_{18}; [540-84-1]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. S. Dubovskaya and M. Kh. Karapetyants, Tr. Inst. - Mosk. Khim.-Tekhnol. Inst. im. D. I. Mendeleeva **58**, 92–7 (1968).

Variables:

T/K=298–303

Compiled by:

A. Skrzecz

8.9. 2-Methyl-2-propanol + Water + 2,2,4-Trimethylpentane

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
0.0	273.2	0.2042	0.7320	0.1515	0.8370
		0.1118	0.8094	0.0811	0.9050
		0.1245	0.7770	0.0925	0.8897
		0.3662	0.4593	0.3280	0.6340
		0.4089	0.4012	0.3810	0.5760
		0.4357	0.3181	0.4420	0.4973
		0.4254	0.2335	0.4900	0.4145
		0.4275	0.2288	0.4950	0.4083
		0.4009	0.1152	0.5760	0.2550
		0.4008	0.1123	0.5790	0.2500
		0.3929	0.0984	0.5880	0.2270
		0.3485	0.0630	0.5920	0.1650
		0.3406	0.0567	0.5930	0.1520
		0.3267	0.0471	0.5925	0.1315
		0.3130	0.0474	0.5780	0.1350
		0.2294	0.0172	0.5225	0.0605
		0.2176	0.0145	0.5100	0.0525
		0.1723	0.0059	0.4520	0.0240
20.0	293.2	0.2042	0.7320	0.1515	0.8370
		0.1118	0.8094	0.0811	0.9050
		0.1245	0.7770	0.0925	0.8897
		0.3662	0.4593	0.3280	0.6340
		0.4089	0.4012	0.3810	0.5760
		0.4254	0.2335	0.4900	0.4145
		0.4275	0.2288	0.4950	0.4083
		0.4398	0.1701	0.5520	0.3290
		0.4291	0.1691	0.5450	0.3310
		0.4282	0.1438	0.5680	0.2940
		0.3993	0.0969	0.5950	0.2225
		0.3335	0.0494	0.5960	0.1360
		0.3260	0.0476	0.5910	0.1330
		0.3158	0.0445	0.5850	0.1270
		0.2694	0.0303	0.5540	0.0960
		0.2138	0.0146	0.5044	0.0531
		0.2084	0.0136	0.4980	0.0500
		0.1726	0.0074	0.4502	0.0298
		0.1274	0.0045	0.3688	0.0202
30.0	303.2	0.1148	0.7986	0.0840	0.9006
		0.1520	0.7469	0.1145	0.8670

0.2721	0.6267	0.2155	0.7650
0.1576	0.7274	0.1206	0.8580
0.4162	0.3618	0.4050	0.5425
0.4385	0.2608	0.4800	0.4400
0.4418	0.1684	0.5550	0.3260
0.4155	0.1027	0.6015	0.2290
0.4126	0.1028	0.5990	0.2300
0.3470	0.0519	0.6055	0.1395
0.3430	0.0509	0.6030	0.1380
0.3492	0.0516	0.6080	0.1385
0.2785	0.0315	0.5630	0.0980
0.2292	0.0196	0.5185	0.0685
0.2162	0.0142	0.5085	0.0515
0.2101	0.0146	0.4990	0.0535
0.1754	0.0075	0.4550	0.0300
0.1501	0.0046	0.4140	0.0195
0.1477	0.0042	0.4100	0.0178
0.1463	0.0044	0.4070	0.0190
0.1376	0.0033	0.3916	0.0144
0.1179	0.0016	0.3526	0.0074
0.1012	0.0004	0.3160	0.0019
0.0883	0.0000	0.2850	0.0000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
30.0	303.2	0.1404	0.7708	0.0269	0.0002	0.1040	0.8800	0.1020	<0.0010
		0.3028	0.5767	0.0381	0.0002	0.2480	0.7280	0.1400	<0.0010
		0.3768	0.4570	0.0456	0.0002	0.3360	0.6280	0.1640	<0.0010
		0.4288	0.2968	0.0560	0.0002	0.4500	0.4800	0.1960	<0.0010
		0.4397	0.1931	0.0636	0.0004	0.5320	0.3600	0.2180	0.0020
		0.4233	0.1205	0.0744	0.0004	0.5880	0.2580	0.2480	0.0020
		0.4098	0.1035	0.0803	0.0002	0.5960	0.2320	0.2640	<0.0010
		0.3891	0.0789	0.0841	0.0002	0.6080	0.1900	0.2740	<0.0010
		0.3560	0.0562	0.0904	0.0002	0.6080	0.1480	0.2900	<0.0010
		0.2829	0.0275	0.1172	0.0009	0.5740	0.0860	0.3520	0.0040
		0.1844	0.0087	0.1844	0.0087	0.468	0.034	0.468	0.034[a]
		0.1839	0.0082	0.1839	0.0082	0.468	0.032	0.468	0.032[b]
		0.1797	0.0055	0.1797	0.0055	0.465	0.022	0.465	0.022[c]

The authors calculated critical points: (a) by Alekseev's, Ref. 1, (b) by Izmailov's, Ref. 2, and (c) by Zilberman's, Ref. 3, methods, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine the solubility curve. Binary hydrocarbon–alcohol mixtures were titrated with water until turbidity was observed, as described in Ref. 4. The titration was repeated several times to eliminate errors. The relationship of density versus composition of saturated mixture was used later to calculate equilibrium. The method was tested on the ethanol–heptane–water system and the results were in agreement with literature data. The analytical method was used to determine liquid–liquid equilibria. A binary mixture of known composition was placed in a special thermostated vessel and the third component was added to obtain a two-phase mixture. This mixture was agitated for 3–4 h to ensure equilibrium. The mixture was allowed to stand 1–2 h to become clear and then both phases were taken for density measurements. On the basis the previously constructed relationship of density versus composition of the saturated mixture, the composition of the mixture in equilibrium was calculated. Concentrations of 2,2,4-trimethylpentane in the water-rich phase were reported in the paper for several experimental points as <0.0010 of mass fraction while the sums of water and alcohol concentrations were equal to 1.0000. Recalculations to mole fraction were made treating them as real values.

Source and Purity of Materials:

(1) source not specified; $d(20\ °C,20\ °C)=0.7894$, $n(25\ °C,D)=1.3860$, m.p. = 25 °C; used as received.
(2) source not specified; $d(20\ °C,20\ °C)=0.6890$, $n(25\ °C,D)=1.3890$.
(3) doubly distilled.

Estimated Error:

temp. ±0.1 K; conc. ±0.0001.

References:

[1] V. F. Alekseev, Gorn. Zh. **2**, 385 (1985).
[2] N. A. Izmajlov and A. K. Franke, Zh. Fiz. Khim. **29**, 120 (1955).
[3] E. N. Zilberman Zh. Fiz. Khim. **28**, 1458 (1952).
[4] W. D. Bancroft, Phys. Rev. **3**, 21 (1896).

Components:

(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0]
(2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12} ; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

8.10. 2-Methyl-2-propanol + Water + Mesitylene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.115	0.003	0.344	0.015
		0.164	0.011	0.429	0.047
		0.224	0.022	0.506	0.081
		0.304	0.047	0.565	0.142
		0.375	0.099	0.565	0.242
		0.413	0.170	0.523	0.349
		0.425	0.262	0.459	0.459
		0.401	0.371	0.379	0.569
		0.349	0.504	0.290	0.680
		0.267	0.660	0.197	0.790
		0.149	0.827	0.100	0.896
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.290	0.615	0.030	0.000	0.221	0.761	0.113	0.000
		0.381	0.430	0.038	0.000	0.339	0.620	0.140	0.000
		0.421	0.228	0.055	0.000	0.481	0.422	0.193	0.000
		0.362	0.088	0.080	0.001	0.567	0.224	0.262	0.005
		0.282	0.041	0.100	0.002	0.550	0.130	0.311	0.010

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by the addition of anhydrous potassium carbonate, distilled; purity better than 99.6 mole % by glc.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1]T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2]S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3]T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:	Original Measurements:
(1) 2-Methyl-2-propanol (tert-butanol, tert-butyl alcohol); $C_4H_{10}O$; [75-65-0] (2) Tetradecane (*n*-tetradecane); $C_{14}H_{30}$; [629-59-4] (3) Water; H_2O; [7732-18-5]	M. K. Silva, M. J. Michnick, and G. P. Willhite, Fluid Phase Equilib. **59**, 247–62 (1990).
Variables: T/K=298	**Compiled by:** A. Skrzecz

8.11. 2-Methyl-2-propanol + Water + Tetradecane

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
25.0	298.2	0.2503	0.6653	0.1415	0.0004	0.122	0.868	0.403	0.003
		0.2533	0.6474	0.1530	0.0008	0.126	0.862	0.424	0.006
		0.2684	0.6335	0.1983	0.0024	0.135	0.853	0.497	0.016
		0.2737	0.6359	0.2038	0.0023	0.137	0.852	0.506	0.015
		0.2786	0.6313	0.2129	0.0025	0.140	0.849	0.519	0.016
		0.2819	0.6282	0.2212	0.0025	0.142	0.847	0.531	0.016
		0.2835	0.6267	0.2229	0.0027	0.143	0.846	0.533	0.017
		0.2922	0.6260	0.2447	0.0033	0.147	0.843	0.561	0.020
		0.2954	0.6230	0.2506	0.0035	0.149	0.841	0.568	0.021
		0.3003	0.6185	0.2602	0.0039	0.152	0.838	0.579	0.023
		0.3019	0.6170	0.2651	0.0039	0.153	0.837	0.585	0.023
		0.3668	0.4529	0.4110	0.0196	0.226	0.747	0.683	0.087
		0.3807	0.4308	0.4306	0.0234	0.241	0.730	0.688	0.100
		0.3974	0.4070	0.4460	0.0289	0.259	0.710	0.685	0.119
		0.4108	0.3818	0.4577	0.0348	0.277	0.689	0.679	0.138
		0.4439	0.3250	0.4834	0.0503	0.324	0.635	0.661	0.184

Comments: Data reported in the above table were adjusted by the compiler so that the sum of mass fractions equaled 1.000, the presented results were always within the authors' 95% confidence interval.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Mixtures containing approximately equal volumes of each phase, in vials capped with teflon-lined septa were vigorously shaken and then allowed to equilibrate at least 24 h in a thermostated water bath. Six to 14 glc analyses[1] with ethanol as the internal standard, were performed on each sample. Reported concentrations of each component were bounded by estimated 95% confidence interval, but the sum of mass fraction differed from 1.000.

Source and Purity of Materials:

(1) Fisher Scientific, certified; used as received; purity >99 wt %, verified by glc.
(2) Aldrich, certified; used as received; purity >99 wt %, verified by glc.
(3) de-ionized and distilled, sodium concentration <0.025 ppm sodium.

Estimated Error:

temp. ±0.1 °C; composition 0.3%–3.0% of the measured value (estimated by the authors).

References:

[1] M. K. Silva, Dissertation, Univ. of Kansas, Lawrence, Kansas, 1990.

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9. 1-Butanol +Water

Components:	Evaluated by:
(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3] (2) Benzene; C_6H_6 ; [71-43-2] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.03)

9.1. 1-Butanol + Water + Benzene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-butanol–benzene–water is given in Table 72.

TABLE 72. Summary of experimental data for the system 1-butanol–benzene–water

Author(s)	T/K	Type of data[a]	Ref.
Perrakis, 1925	292	sat. (10)	1
Washburn and Strandskov, 1944	298, 308	sat. (20), eq. (28)	2
Staveley *et al.*, 1951	287–333	sat. (28)	3
Letcher *et al.*, 1990	298	sat. (14), eq. (3)	4

[a] Number of experimental points in parentheses.

Saturation curve

The system 1-butanol–benzene–water forms a miscibility gap of type 2. Two binary systems, 1-butanol–water and benzene–water are partially miscible. The data of these systems were compiled and critically evaluated in previously published SDS volumes, Refs. 5 and 6, respectively. Data on the saturation curve of the organic-rich phase were presented in all four references, while data for the water-rich phase were presented only in Ref. 2 as saturation compositions and as a part of equilibrium data. Data of Letcher *et al.*[4] were presented in graphical form only and therefore are not presented here as a compilation sheet. The data of Staveley *et al.*[3] show the relationship of saturation composition to temperature; the data describe the region of low 1-butanol concentrations (<0.1 mole fraction) and high benzene concentrations (>0.88 mole fraction). The paper of Peraksis[1] at 292 K reports a much smaller solubility gap than other data sets at slightly higher temperatures. This paper also reports outlying results for other alcohol–benzene–water systems and therefore these data are rejected and not compiled. The other data sets are treated as tentative. The temperature of 298.2 K as a standard temperature in which various alcohol–hydrocarbon–water systems are presented, was chosen to present the behavior of the system in Fig. 38. The recommended values of mutual solubility at 298.2 K are: $x_2'=0.9970$ and $x_2''=0.000\,409$ for benzene–water system[5] and $x_1'=0.488$, $x_1''=0.0191$ for 1-butanol–water.[6] The maximum 1-butanol concentration in organic-rich phase of this ternary system was observed to be $x_1=0.532$, Ref. 2; similar values were presented as a graph in Ref. 4. The water-rich phase compositions are very closed to the side of concentration triangle diagram and are consistent with recommended binary data.[5,6]

Phases in equilibrium

Compositions of coexisting phases in equilibrium of the ternary 1-butanol–benzene–water system were reported by Washburn and Strandskov[2] at 298.2 K and 308 K and cover the whole range of the miscibility gap. Graphical data of Letcher *et al.*[4] at 298 K were not taken into account. The tie lines are consistent within each data set and are consistent with one another. Both equilibrium data sets are treated as tentative. The experimental tie lines at 298.2 K, are presented in Fig. 38.

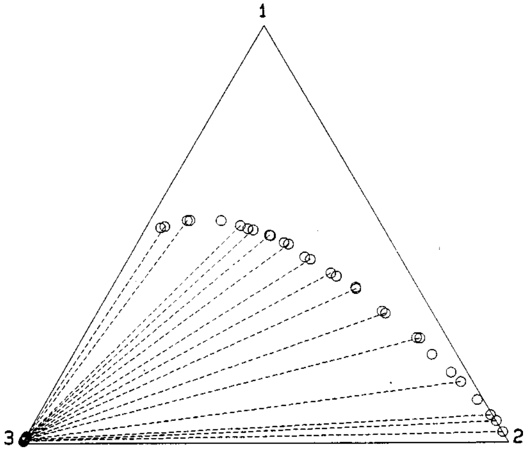

FIG. 38. Phase diagram of the system 1-butanol (1)—benzene (2)—water (3) at 298.2 K. ○—experimental data, Ref. 2, dashed lines—experimental tie lines, Ref. 2.

References:

[1] N. Perrakis, J. Chem. Phys. **22**, 280 (1925).

[2] E. R. Washburn and C. V. Strandskov, J. Phys. Chem. **48**, 241 (1944).

[3] L. A. K. Staveley, R. G. S. Johns, and B. C. Moore, J. Chem. Soc. 2516 (1951).

[4] T. M. Letcher, J. Sewry, and S. Radloff, S. Afr. J. Chem. **43**, 56 (1990).

[5] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[6] A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. R. Washburn and C. V. Strandskov, J. Phys. Chem. **48**, 241–5 (1944).

Variables:

T/K=298 and 308

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)			
25.0	298.15	0.1025	0.8843	0.0988	0.8981
		0.1685	0.7976	0.1656	0.8263
		0.2120	0.7362	0.2119	0.7755
		0.2518	0.6848	0.2546	0.7298
		0.3152	0.5820	0.3306	0.6432
		0.3724	0.4991	0.4006	0.5658
		0.3987	0.4464	0.4397	0.5188
		0.4445	0.3586	0.5108	0.4342
		0.4789	0.2995	0.5645	0.3720
		0.4956	0.2640	0.5955	0.3343
		0.5121	0.2095	0.6397	0.2758
		0.5312	0.1456	0.6960	0.2011
		0.5323	0.0810	0.7480	0.1199
		0.5147	0.0294	0.7840	0.0472
		0.0090	0.0007	0.0358	0.0030
		0.0059	0.0005	0.0237	0.0020
35.0	308.15	0.0708	0.9168	0.0681	0.9290
		0.1165	0.8640	0.1129	0.8825
		0.1665	0.8032	0.1632	0.8296
		0.2356	0.7017	0.2379	0.7467
		0.3243	0.5777	0.3389	0.6362
		0.3748	0.4881	0.4063	0.5576
		0.4097	0.4146	0.4607	0.4913
		0.4722	0.2946	0.5626	0.3699
		0.4892	0.2373	0.6071	0.3104
		0.5127	0.1475	0.6829	0.2071
		0.5130	0.0757	0.7406	0.1151
		0.5045	0.0324	0.7747	0.0525
		0.0129	0.0007	0.0508	0.0028
		0.0047	0.0004	0.0190	0.0018

Compositions of coexisting phases

$t/°C$	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25.0	298.15	0.0253	0.9747	0.0047	0.0005	0.024	0.976	0.019	0.002
		0.0515	0.9485	0.0062	0.0005	0.049	0.951	0.025	0.002
		0.0659	0.9297	0.0072	0.0005	0.063	0.936	0.029	0.002
		0.2505	0.6923	0.0095	0.0007	0.252	0.734	0.038	0.003
		0.3102	0.5914	0.0103	0.0007	0.324	0.651	0.041	0.003
		0.3687	0.5014	0.0114	0.0010	0.397	0.569	0.045	0.004
		0.4059	0.4312	0.0124	0.0007	0.451	0.505	0.049	0.003
		0.4390	0.3732	0.0127	0.0010	0.500	0.448	0.050	0.004
		0.4750	0.3105	0.0135	0.0007	0.556	0.383	0.053	0.003
		0.4966	0.2608	0.0140	0.0007	0.598	0.331	0.055	0.003
		0.5091	0.2216	0.0148	0.0007	0.630	0.289	0.058	0.003
		0.5197	0.1907	0.0153	0.0007	0.657	0.254	0.060	0.003
		0.5316	0.0758	0.0164	0.0007	0.752	0.113	0.064	0.003
		0.5177	0.0366	0.0172	0.0005	0.779	0.058	0.067	0.002
35.0	308.15	0.0376	0.9538	0.0042	0.0005	0.036	0.962	0.017	0.002
		0.0890	0.8939	0.0067	0.0007	0.086	0.910	0.027	0.003
		0.1568	0.8179	0.0077	0.0007	0.153	0.841	0.031	0.003
		0.2128	0.7338	0.0088	0.0005	0.213	0.774	0.035	0.002
		0.2813	0.6423	0.0095	0.0005	0.288	0.693	0.038	0.002
		0.3309	0.5708	0.0100	0.0007	0.346	0.629	0.040	0.003
		0.3842	0.4725	0.0111	0.0007	0.419	0.543	0.044	0.003
		0.4340	0.3720	0.0116	0.0007	0.497	0.449	0.046	0.003
		0.4642	0.3154	0.0124	0.0007	0.546	0.391	0.049	0.003
		0.4826	0.2637	0.0129	0.0007	0.587	0.338	0.051	0.003
		0.5029	0.1924	0.0134	0.0005	0.645	0.260	0.053	0.002
		0.5135	0.1334	0.0148	0.0005	0.694	0.190	0.058	0.002
		0.5102	0.0475	0.0166	0.0000	0.764	0.075	0.065	0.000

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities were determined by titration of weighed solutions to permanent appearance of a second phase. Observations were made with both reflected and transmitted light and against a light or dark background. The titrant was added from a pipet which ended with in fine capillary; the amount added was determined by weight. The total mass of the mixture was 18–25 g. Refractive indexes of saturated solutions were measured and plotted as a function of concentration. Tie-lines were determined by adding alcohol in varying amounts to binary water–benzene mixtures. After separation, refractive indexes of conjugate layers were determined and the concentrations were read from the plots.

Source and Purity of Materials:

(1) Eastman Kodak Co., better grade; dried by refluxing over active lime, distilled; $d(25\ °C, 4\ °C) = 0.806\ 49$.
(2) Coleman and Bell, reagent quality grade; dried with Na, crystallized several times; f.p. = 5.45 °C.
(3) doubly distilled over $KMnO_4$.

Estimated Error:

temp. ±0.05 °C.

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. A. K. Staveley, R. G. S. Johns, and B. C. Moore, J. Chem. Soc. 2516–23 (1957).

Variables:

$T/K = 286–333$

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°C$	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
24.7	297.85	0.008 02	0.988 708	0.007 633	0.991 611
32.6	305.75	0.008 02	0.987 635	0.007 639	0.991 355
42.3	315.45	0.008 02	0.985 953	0.007 649	0.990 954
51.5	324.65	0.008 02	0.983 756	0.007 662	0.990 429
16.8	289.95	0.014 05	0.982 584	0.013 376	0.985 845
35.6	308.75	0.014 05	0.979 741	0.013 406	0.985 154
45.1	318.25	0.014 05	0.977 894	0.013 425	0.984 704
54.2	327.35	0.014 05	0.975 570	0.013 449	0.984 136
18.8	291.95	0.026 15	0.969 185	0.024 937	0.973 982
26.8	299.95	0.026 15	0.968 104	0.024 958	0.973 709
35.0	308.15	0.026 15	0.966 882	0.024 981	0.973 401
44.0	317.15	0.026 15	0.965 339	0.025 011	0.973 010
51.9	325.05	0.026 15	0.963 580	0.025 045	0.972 564
14.8	287.95	0.0329	0.961 345	0.031 411	0.967 254
26.4	299.55	0.0329	0.960 018	0.031 443	0.966 912
34.3	307.45	0.0329	0.959 035	0.031 467	0.966 658
45.9	319.05	0.0329	0.957 355	0.031 508	0.966 223
57.9	331.05	0.0329	0.955 300	0.031 559	0.965 690
12.6	285.75	0.0561	0.935 951	0.053 716	0.944 434
24.1	297.25	0.0561	0.934 520	0.053 776	0.944 039
35.9	309.05	0.0561	0.932 89	0.053 844	0.943 587
47.2	320.35	0.0561	0.931 23	0.053 914	0.943 127
60.2	333.35	0.0561	0.929 23	0.053 998	0.942 570
13.8	286.95	0.0973	0.890 40	0.093 681	0.903 441
24.3	297.45	0.0973	0.888 51	0.093 820	0.902 855
35.6	308.75	0.0973	0.886 45	0.093 971	0.902 215
46.8	319.95	0.0973	0.884 33	0.094 127	0.901 554
59.5	332.65	0.0973	0.881 73	0.094 320	0.900 740

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Mixtures were prepared in a closed apparatus; components were degassed by repeated freezing, evacuation, and melting; a known amount of each component was introduced into a tube by condensation and the tube was sealed. The volume of each tube was about 30 mL.

Source and Purity of Materials:

(1) source not specified; dried by refluxing over freshly ignited lime, and then with aluminum amalgam, distilled. (1) source not specified; used as received.
(2) source not specified; chemically purified, crystallized, distilled, dried over phosphoric anhydride.
(3) not specified.

Estimated Error:

composition <0.2%; temp. <0.2 °C.

Components:	**Evaluated by:**
(1) 1-Butanol (*n*-butanol; butyl alcohol; *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3] (2) Cyclohexane; C_6H_{12} ; [110-82-7] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1995.09)

9.2. 1-Butanol + Water + Cyclohexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-butanol–cyclohexane–water is given in Table 73.

TABLE 73. Summary of experimental data for the system 1-butanol–cyclohexane–water

Author(s)	T/K	Type of data[a]	Ref.
Plackov and Stern, 1990	298	sat. (13), eq. (6)	1
Letcher *et al.*, 1991	298	sat. (14), eq. (5)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 1-butanol–cyclohexane–water forms a miscibility gap of type 2. The system was studied by titration method at 298.2 K in both cases. Two binary systems, cyclohexane–water and 1-butanol–water, form miscibility gaps. The data of these binary systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. The recommended values of mutual solubility at 298 K are: for cyclohexane–water system $x_2''=1.2\cdot 10^{-5}$ and $x_3'=3.7\cdot 10^{-4}$,[3] and for 1-butanol–water system $x_1'=0.488$ and $x_1''=0.0191$.[4] Letcher *et al.*[2] reported ternary data and the mutual solubility of the binary systems. The end points of the saturation curve were reported to be $x_2=0.999$ and pure water which is inconsistent with recommended values but within the accuracy of experimental measurements (0.001 mole fraction) stated by the authors. Binary solubility data of the 1-butanol–water system reported in Ref. 2 as $x_1=0.488$ and $x_1=0.019$ were consistent with the ''best values'' reported in the critical evaluation, Ref. 3. Plackov and Stern[1] reported the solubility of 1-butanol in water to be $x_1''=0.0187$. This result is also consistent with recommended data. These experimental data are consistent with one another. Compositions of the water-rich phase of the ternary system, Refs. 1 and 2, were reported as binary 1-butanol–water mixtures; the analytical methods used could not detect cyclohexane. Therefore the water-rich branch cannot be evaluated. Phase equilibrium data were included with the description of the saturation curve of the organic-rich phase and data at 298.2 K were described by the equation:

$$x_1=0.695\,74+0.046\,03\ \ln(x_2)-0.440\,62x_2-0.259\,44x_2^2.$$

The model applies to the region $0.02<x_2<0.99$. The parameters were calculated by the least-squares method. The standard error of estimate was 0.0043. The points on the saturation curve calculated by the above equation for selected concentrations of cyclohexane in the mixture are presented in Table 74 and in Fig. 39 as a calculated binodal curve (solid line).

TABLE 74. Calculated compositions along the saturation curve at 298.2 K (organic-rich phase)

x_1	x_2	x_1	x_2
0.488	0.000 Ref. 4	0.3538	0.5400
0.5068	0.0200	0.3409	0.5600
0.5295	0.0400	0.3278	0.5800
0.5389	0.0600	0.3145	0.6000
0.5426	0.0800	0.3008	0.6200
0.5431	0.1000	0.2869	0.6400
0.5415	0.1200	0.2728	0.6600
0.5385	0.1400	0.2584	0.6800
0.5342	0.1600	0.2438	0.7000
0.5291	0.1800	0.2289	0.7200
0.5232	0.2000	0.2138	0.7400
0.5166	0.2200	0.1984	0.7600
0.5094	0.2400	0.1828	0.7800
0.5016	0.2600	0.1669	0.8000
0.4934	0.2800	0.1508	0.8200
0.4848	0.3000	0.1345	0.8400
0.4757	0.3200	0.1180	0.8600
0.4663	0.3400	0.1012	0.8800
0.4565	0.3600	0.0842	0.9000
0.4463	0.3800	0.0669	0.9200
0.4358	0.4000	0.0495	0.9400
0.4250	0.4200	0.0318	0.9600
0.4139	0.4400	0.0138	0.9800
0.4024	0.4600	0.0048	0.9900
0.3907	0.4800	0.0000	0.99963 Ref. 3
0.3787	0.5000	0.0000	0.000012 Ref. 3
0.3664	0.5200	0.0191	0.0000 Ref. 4

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 1-butanol–cyclohexane–water were reported in two references at 298.2 K by similar experimental procedures. First equilibrium was reached, then the phases were separated and the composition of each was determined. Compositions of the water-rich phase in equilibrium were reported as binary 1-butanol–water mixtures; the analytical methods could not detect cyclohexane. The tie lines cover the whole area of the miscibility gap and they are consistent within each data set. Distribution of 1-butanol differs between data sets with Letcher *et al.*[2] reporting lower concentrations of alcohol in the water-rich phase than the data of Plackov and Stern.[1] The data become similar only in the area of low cyclohexane concentrations ($x_2'<0.090$ in the organic-rich phase). Both data sets are treated as tentative. All experimental data points at 298.2 K are shown in Fig. 39.

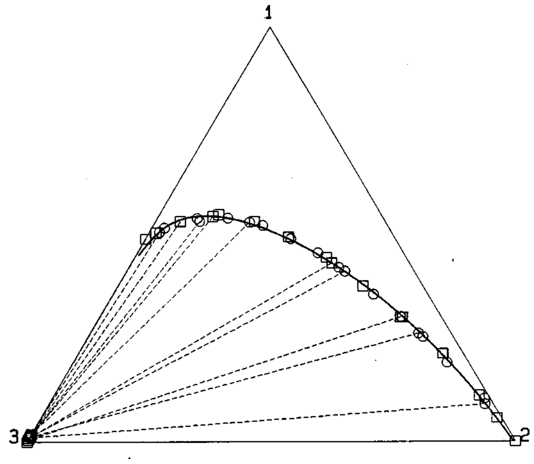

FIG. 39. Phase diagram of the system 1-butanol (1)—cyclohexane (2)—water (3) at 298.2 K. Solid line—calculated binodal curve, ○—experimental results of Ref. 1, □—experimental results of Ref. 2, dashed lines—experimental tie lines, Refs. 1 and 2.

References:

[1] D. Plackov and I. Stern, Fluid Phase Equilib. **57,** 327 (1990).

[2] T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44,** 118 (1991).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[4] A. F. M. Barton, ed., *Solubility Data Series,* Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. Plackov, and I. Stern, Fluid Phase Equilib. **57**, 327–40 (1990).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/ °C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
25.00	298.15	0.1028	0.8853	0.0925	0.9049
		0.1899	0.7657	0.1775	0.8125
		0.2526	0.6851	0.2416	0.7439
		0.3008	0.6153	0.2950	0.6851
		0.3553	0.5324	0.3599	0.6124
		0.4204	0.4290	0.4453	0.5159
		0.4552	0.3686	0.4966	0.4566
		0.4889	0.2958	0.5574	0.3829
		0.5204	0.2228	0.6226	0.3027
		0.5381	0.1425	0.6921	0.2081
		0.5371	0.0806	0.7444	0.1268
		0.5143	0.0251	0.7855	0.0435
		0.0187	0.0000	0.0727	0.0000

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.00	298.15	0.089	0.893	0.010	0.000	0.080	0.916	0.040	0.000
		0.261	0.672	0.012	0.000	0.251	0.733	0.048	0.000
		0.411	0.446	0.013	0.000	0.432	0.532	0.051	0.000
		0.528	0.192	0.015	0.000	0.649	0.268	0.059	0.000
		0.530	0.089	0.016	0.000	0.732	0.140	0.063	0.000
		0.504	0.020	0.018	0.000	0.785	0.035	0.070	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, as reported in Ref. 1, was used to determine the solubility curve. Mixtures of known composition, stirred magnetically and placed in a temperature controlled double-wall Erlenmayer flask, were titrated with the less soluble component until the appearance of turbidity. The analytical method was used to determine liquid–liquid equilibria. The mixture was shaken for at least 20 min. Equilibration took place in a thermostated double-walled separatory funnel of 250 mL over 2 h. The refractive index and density of both phases were measured. The composition was calculated from the calibration data by polynomial regression analysis. Third order polynomials were used. Each experiment was repeated three times.

Source and Purity of Materials:

(1) Zorka (Sabac), analytical grade; used as received; $n=1.3972$, $\rho(25\ °C)=805.9\ kg\ m^{-3}$, b.p.=117.4 °C.
(2) Kemika (Zagreb), analytical grade; used as received; $n=1.4232$, $\rho(25\ °C)=773.6\ kg\ m^{-3}$, b.p.=80.0 °C.
(3) double distilled in the presence of $KMnO_4$.

Estimated Error:

temp. ±0.02 °C; composition $<\pm0.05\%$ (by mass) relative error.

References:

[1] E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transuel, J. Am. Chem. Soc. **62**, 1454 (1940).

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Cyclohexane; C_6H_{12}; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118–21 (1991).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental values:

Compositions along the saturation curve

t/ °C (compiler)	T/K	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.019	0.000	0.074	0.000
		0.488	0.000	0.797	0.000
		0.502	0.014	0.790	0.025
		0.546	0.120	0.715	0.178
		0.530	0.201	0.644	0.277
		0.493	0.289	0.564	0.375
		0.444	0.392	0.478	0.479
		0.375	0.501	0.385	0.584
		0.300	0.620	0.293	0.688
		0.212	0.746	0.198	0.792
		0.110	0.871	0.100	0.896
		0.056	0.934	0.050	0.948
		0.000	0.999	0.0000	0.9998

Compositions of coexisting phases

t/ °C (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.488	0.000	0.019	0.000	0.797	0.000	0.074	0.000
		0.530	0.050	0.016	0.000	0.769	0.082	0.063	0.000
		0.542	0.110	0.014	0.000	0.721	0.166	0.055	0.000
		0.431	0.409	0.009	0.000	0.461	0.497	0.036	0.000
		0.300	0.615	0.005	0.000	0.294	0.685	0.020	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the titration method, as described in Ref. 1. The formation of a cloudy mixture was observed visually on shaking after addition of a known mass of the third component; syringes were precisely weighted. Tie line compositions were determined by the refractive index method, Ref. 2, and a complementary method using the Karl Fischer titration, Ref. 3. Measurements were made at pressure of 94.7 kPa.

Source and Purity of Materials:

(1) Merck; AR grade; dried by addition of anhydrous K_2CO_3, distilled; purity >99.9 mole % by glc.
(2) BDH; Gold label grade; used as received; purity >99.9 mole % by glc.
(3) not specified.

Estimated Error:

composition ±0.005 mole fraction (binodal curve), ±0.01 mole fraction (tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:	**Evaluated by:**
(1) 1-Butanol (*n*-butanol; butyl alcohol; *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3] (2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1995.09)

9.3. 1-Butanol + Water + Hexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-butanol–hexane–water is given in Table 75.

TABLE 75. Summary of experimental data for the system 1-butanol–1-hexane–water

Author(s)	T/k	Type of data[a]	Ref.
Sugi and Katayama, 1977	298	sat. (15), eq. (7)	1
Morozov *et al.*, 1978	333	sat. (7)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 1-butanol–hexane–water forms a miscibility gap of type 2. The system was studied by the titration method in both cases and is presented below at 298.2 K. Two binary systems, hexane–water and 1-butanol–water, form miscibility gaps. The data for these binary systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. The recommended values of mutual solubility at 298 K are: for hexane–water system $x_2''=2.3\cdot 10^{-6}$ and $x_2'=0.999\,53$, Ref. 3, and for 1-butanol–water system $x_1'=0.488$ and $x_1''=0.0191$, Ref. 4. The solubility of water in hexane, reported by Sugi and Katayama[1] ($x_2'=0.99949$) is consistent with recommended value of Ref. 3, while mutual solubility of 1-butanol–water system ($x_1''=0.0151$ and $x_1'=0.5032$) differ a little from recommended data, Ref. 4. Both data sets measured at various temperatures are mutually consistent and are treated as tentative. Compositions of water-rich phase were reported as hexane free in Ref. 1 and therefore this branch cannot be evaluated. The organic-rich phase data of Ref. 1 (saturation and equilibrium data together) were described by the equation:

$$x_1=0.694\,76+0.046\,08\ln(x_2)-0.404\,41x_2-0.283\,19x_2^2.$$

The model applies to the region $0.03<x_2<0.86$, as data reported in Ref. 1. The parameters were calculated by the least-squares method. The standard error of estimate was 0.0017. The points on the saturation curve calculated by the above equation for selected concentrations of hexane in the mixture are presented in Table 76 and in Fig. 40 as a calculated binodal curve (solid line).

TABLE 76. Calculated compositions along the saturation curve at 298.2 K.

x_1	x_2	x_1	x_2
0.488	0.000 Ref. 4	0.4016	0.4800
0.5208	0.0300	0.3898	0.5000
0.5298	0.0400	0.3778	0.5200
0.5398	0.0600	0.3654	0.5400
0.5442	0.0800	0.3528	0.5600
0.5454	0.1000	0.3398	0.5800
0.5445	0.1200	0.3266	0.6000
0.5420	0.1400	0.3131	0.6200
0.5384	0.1600	0.2994	0.6400
0.5338	0.1800	0.2853	0.6600
0.5284	0.2000	0.2710	0.6800
0.5223	0.2200	0.2565	0.7000
0.5156	0.2400	0.2416	0.7200
0.5084	0.2600	0.2265	0.7400
0.5007	0.2800	0.2112	0.7600
0.4925	0.3000	0.1956	0.7800
0.4838	0.3200	0.1797	0.8000
0.4748	0.3400	0.1636	0.8200
0.4654	0.3600	0.1472	0.8400
0.4556	0.3800	0.1306	0.8600
0.4455	0.4000	0.0000	0.99953 Ref. 3
0.4350	0.4200	0.0000	$2.3\cdot10^{-6}$ Ref. 3
0.4242	0.4400	0.0191	0.0000 Ref. 4
0.4130	0.4600		

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 1-butanol–hexane–water were reported only by Sugi and Katayama.[1] Concentration of hexane in the water-rich phase in equilibrium was assumed to be 0.0. The tie lines cover the whole area of the miscibility gap and are consistent within data set. Consequently they are treated as tentative. All experimental data points at 298.2 K are shown in Fig. 40.

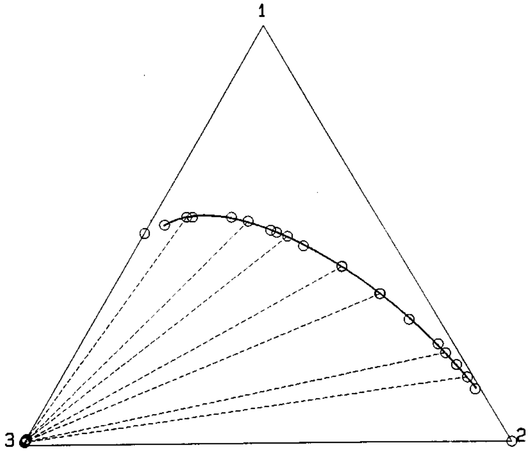

FIG. 40. Phase diagram of the system 1-butanol (1)—hexane (2)—water (3) at 298.2 K. Solid line—calculated binodal curve, ○—experimental results of Ref. 1, dashed lines—experimental tie lines, Ref. 1.

References:

[1] H. Sugi and T. Katayama, J. Chem. Eng. Jpn. **10**, 400 (1977).

[2] A. V. Morozov, A. G. Sarkisov, V. B. Turovskii, and V. I. Ilyaskin, Dep. Doc. VINITI **102–78**, 1 (1978).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[4] A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 1-Butanol (*n*-butanol; butyl alcohol; *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

H. Sugi and T. Katayama, J. Chem. Eng. Jpn. **10**, 400-2 (1977).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.0000	0.99949	0.0000	0.99989
		0.1255	0.8630	0.1109	0.8866
		0.1839	0.7960	0.1650	0.8306
		0.2337	0.7342	0.2134	0.7795
		0.2928	0.6459	0.2766	0.7093
		0.3548	0.5557	0.3470	0.6318
		0.4220	0.4460	0.4339	0.5331
		0.4709	0.3427	0.5148	0.4356
		0.5035	0.2714	0.5763	0.3611
		0.5091	0.2560	0.5894	0.3446
		0.5407	0.1598	0.6765	0.2324
		0.5413	0.0792	0.7460	0.1269
		0.5229	0.0310	0.7835	0.0540
		0.5032	0.0000	0.8065	0.0000
		0.0151	0.0000	0.0593	0.0000

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.1540	0.8328	0.0066	0.0000	0.1368	0.8603	0.0266	0.0000
		0.2118	0.7601	0.0071	0.0000	0.1921	0.8017	0.0286	0.0000
		0.3547	0.5571	0.0080	0.0000	0.3464	0.6326	0.0321	0.0000
		0.4207	0.4460	0.0090	0.0000	0.4330	0.5337	0.0360	0.0000
		0.4942	0.2983	0.0102	0.0000	0.5544	0.3890	0.0407	0.0000
		0.5311	0.1989	0.0120	0.0000	0.6414	0.2793	0.0476	0.0000
		0.5413	0.0669	0.0129	0.0000	0.7578	0.1089	0.0510	0.0000

Auxiliary Information

Method/Apparatus/Procedure:

A combination of a titration and analytical method was used. The apparatus and experimental procedure were described in Ref. 1. For glc analysis a 1.6 m column filled with Poropak-Q was used. Solubility of water in hexane was determined by the Karl Fischer method. Composition of the water-rich phase was determined by the gross composition of phase split liquid mixture and composition of the organic phase (concentration of hexane was assumed to be 0).

Source and Purity of Materials:

(1) Merck Uvasol, spectrograde; used as received; densities agreed within 0.0003 with literature values.
(2) Merck Uvasol, spectrograde; used as received; densities agreed within 0.0003 with literature values.
(3) de-ionized, twice distilled.

Estimated Error:

Not reported.

References:

[1] H. Sugi, T. Nitta, and T. Katayama, J. Chem. Eng. Jpn. **9**, 12 (1976).

Components:	**Original Measurements:**
(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3] (2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3] (3) Water; H_2O; [7732-18-5]	A. V. Morozov, A. G. Sarkisov, V. B. Turovskii, and V. I. Ilyaskin, Dep. Doc. VINITI **102-78,** 1–9 (1978).
Variables:	**Compiled by:**
$T/\mathrm{K}=333$	A. Skrzecz

Experimental Data

Compositions along the saturation curve

$t/°\mathrm{C}$	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
60	333.2	0.4875	0.0425	0.7487	0.0759
		0.4890	0.0469	0.7451	0.0831
		0.5055	0.1087	0.6966	0.1742
		0.4980	0.1840	0.6310	0.2711
		0.4193	0.3607	0.4700	0.4701
		0.2902	0.5827	0.2906	0.6784
		0.1010	0.8340	0.0930	0.8925

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. The composition of the organic-rich phase was presented; the composition of the water-rich phase was not investigated.

Source and Purity of Materials:

(1) source not specified; dried, distilled, $n(20\ °\mathrm{C,D})=1.3991$, $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.8010$.
(2) source not specified; twice distilled, $n(20\ °\mathrm{C,D})=1.3748$, $d(25\ °\mathrm{C},4\ °\mathrm{C})=0.6544$.
(3) doubly distilled.

Estimated Error: Not reported.

Components:	**Evaluated by:**
(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3] (2) Toluene (methylbenzene); C_7H_8; [108-88-3] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.12)

9.4. 1-Butanol + Water + Toluene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-butanol–toluene–water is given in Table 77.

TABLE 77. Summary of experimental data for the system 1-butanol–toluene–water

Author(s)	T/k	Type of data[a]	Ref.
Fuoss, 1943	303	sat. (27), eq. (14)	1
Shanahan, 1948	293	sat. (5)	2
Letcher and Siswana, 1992	298	sat. (15). eq. (5)	3

[a] Number of experimental points in parenthescs.

Saturation curve

The system 1-butanol–toluene–water forms a miscibility gap of type 2. Two binary systems, 1-butanol–water and toluene–water, are partially miscible. The data of these systems were compiled and critically evaluated in previously published SDS volumes, Refs. 4 and 5, respectively. The recommended values of mutual solubility at 298.2 K are: $x_2'=0.9972$, $x_2''=0.000\ 104$ for toluene–water system[4] and $x_1'=0.488$, $x_1''=0.0191$ for 1-butanol–water.[5] The saturation curve for the organic-rich phase was measured by Fuoss[1] by the conductance method; the water-rich phase was assumed to be toluene free. Shanahan[2] measured only the saturation curve at 293 K. Letcher and Siswana reported both saturation and equilibrium results at 298 K. Each of these reported measurements was made at a different temperature and therefore no recommendation can be made. However, all these data are consistent with one another. All three data sets are treated as tentative. The maximum 1-butanol concentration was observed in the organic-rich branch of the saturation curve at each reported temperatures, in the area of $x_1=0.54\pm0.01$ and $x_2=0.11\pm0.02$. The saturation mixtures of the water-rich branch contained undetectably small amounts of toluene; the water-rich phase was reported as a binary 1-butanol–water mixture by both Refs. 1 and 3. The temperature of 298 K was chosen for graphical presentation and therefore only experimental data of Letcher and Siswana[3] are shown in Fig. 41. The binary data reported with ternary data sets are in agreement with the previously recommended binary solubility data.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary 1-butanol–toluene–water system were reported in Refs. 1 and 3, at 303 and 298 K respectively, and cover the whole range of the miscibility gap. The tie lines are consistent within each data set, but the data sets are inconsistent with one another because tie lines cross. It is unlikely that a temperature difference of 5 K gives such large changes in phase composition e.g., water-rich phase $x_1=0.007$ in equilibrium with organic-rich phase $x_1=0.341$, $x_2=0.570$ at $T/\mathrm{K}=298$, Ref. 3; and water-rich phase $x_1=0.0063$ in equilibrium with organic-rich phase $x_1=0.0609$, $x_2=0.9291$ at $T/\mathrm{K}=303$, Ref. 1. Both equilibrium data sets are treated as tentative. The experimental tie lines at 298 K by Letcher and Siswana, Ref. 3, are presented in Fig. 41.

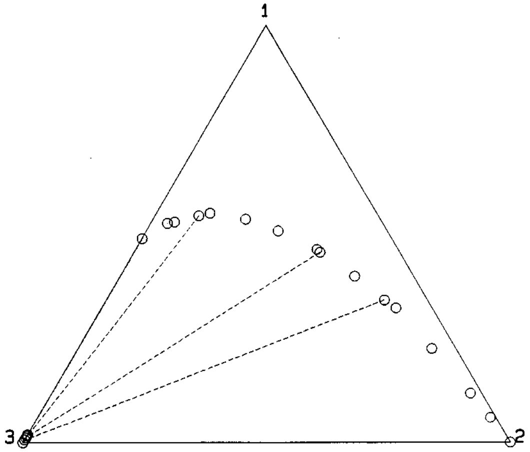

FIG. 41. Phase diagram of the system 1-butanol (1)—toluene (2)—water (3) at 298.2 K. ○—experimental data, Ref. 3, dashed lines—experimental tie lines, Ref. 3.

References:

[1] R. M. Fuoss, J. Am. Chem. Soc. **65**, 78 (1943).

[2] C. E. A. Shanahan, Analyst (London) **73**, 502 (1948).

[3] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

[4] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[5] A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

R. M. Fuoss, J. Am. Chem. Soc. **65**, 78–81 (1943).

Variables:

T/K=303

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

	T/K	x_1	x_2			
t/ °C	(compiler)	(compiler)		w_1	w_2	
30.0	303.15	0.2231	0.7228	0.1966	0.7918	set A
		0.2260	0.7186	0.1995	0.7886	
		0.3874	0.4745	0.3833	0.5835	
		0.4696	0.3221	0.5101	0.4349	
		0.5131	0.2136	0.6072	0.3142	
		0.5299	0.1384	0.6771	0.2199	
		0.5280	0.0736	0.7371	0.1277	
		0.5151	0.0339	0.7724	0.0632	
		0.4834	0.0000	0.7938	0.0000	
30.0	303.15	0.0884	0.8981	0.0732	0.9241	set B
		0.2244	0.7219	0.1977	0.7908	
		0.3897	0.4701	0.3865	0.5797	
		0.4961	0.2668	0.5603	0.3746	
		0.5284	0.1444	0.6711	0.2279	
		0.5204	0.0465	0.7614	0.0846	
		0.4834	0.0000	0.7938	0.0000	
30.0	303.15	0.0884	0.8981	0.0732	0.9241	set C
		0.1742	0.7908	0.1494	0.8433	
		0.2238	0.7202	0.1976	0.7904	
		0.3008	0.6252	0.2745	0.7091	
		0.3526	0.5317	0.3385	0.6345	
		0.4525	0.3571	0.4800	0.4709	
		0.4946	0.2647	0.5607	0.3730	
		0.5166	0.2025	0.6175	0.3009	
		0.5300	0.1406	0.6753	0.2227	
		0.5323	0.1079	0.7061	0.1779	
		0.5257	0.0625	0.7473	0.1104	
		0.5016	0.0213	0.7788	0.0412	
		0.4834	0.0000	0.7938	0.0000	

Compositions of coexisting phases

t/ °C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		Organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
30.0	303.15	0.012	0.988	0.0021	0.0000	0.010	0.990	0.0085	0.0000
		0.025	0.975	0.0038	0.0000	0.020	0.980	0.0155	0.0000
		0.037	0.963	0.0049	0.0000	0.030	0.970	0.0200	0.0000
		0.049	0.946	0.0058	0.0000	0.040	0.959	0.0235	0.0000
		0.061	0.929	0.0063	0.0000	0.050	0.948	0.0255	0.0000
		0.119	0.861	0.0080	0.0000	0.100	0.896	0.0320	0.0000
		0.226	0.718	0.0094	0.0000	0.200	0.788	0.0375	0.0000
		0.319	0.580	0.0104	0.0000	0.300	0.677	0.0415	0.0000
		0.401	0.455	0.0115	0.0000	0.400	0.565	0.0455	0.0000
		0.463	0.332	0.0126	0.0000	0.500	0.446	0.0500	0.0000
		0.509	0.220	0.0137	0.0000	0.600	0.322	0.0540	0.0000
		0.531	0.114	0.0149	0.0000	0.700	0.186	0.0585	0.0000
		0.519	0.056	0.0162	0.0000	0.750	0.101	0.0635	0.0000
		0.484	0.000	0.0182	0.0000	0.794	0.000	0.0710	0.0000

Auxiliary Information

Method/Apparatus/Procedure:

The conductance method (set A) was used to obtain compositions along the saturation curve. Weighed mixtures of about 150 g of toluene and butanol in glass-stoppered Erlenmeyer flasks were placed in a thermostat and portions of water, containing a trace ($<0.5\%$) of HCl, were added. As long as water dissolves in the organic phase, its conductance increases. With the appearance of an aqueous phase the conductance of the organic phase drops on further addition of water, because the aqueous phase extracts HCl from the organic phase. Set B and set C present the compositions of the saturated organic phase used for refractive index (on an Abbe refractometer) and density (in 25 mL pyknometer) measurements. The refractive index and density of binary butanol–water mixtures were measured in similar way. Solubility of toluene in the butanol–water mixture was estimated to be about 0.03% and its effect on density and refractive index of aqueous phase was assumed to be negligible. Large scale plots of composition functions for refractive index and density were used to determine the compositions of phases in equilibrium. To determine equilibrium, the mixtures of three components were shaken together and after separation samples of both phases were taken for density and refractive index measurements.

Source and Purity of Materials:

(1) source not specified, c.p. products; distilled; densities and refractive indexes were in agreement with ‘‘International Critical Tables’’.
(2) source not specified, c.p. product; distilled; densities and refractive indexes were in agreement with ‘‘International Critical Tables’’.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

C. E. A. Shanahan, Analyst (London) **73**, 502–3 (1948).

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/ °C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
20	293.15	0.4950	0.0000	0.8013	0.0000
	293.15	0.5314	0.1518	0.6667	0.2367
	293.15	0.4439	0.3807	0.4625	0.4931
	293.15	0.2605	0.6710	0.2344	0.7506
	293.15	0.0000	0.9949	0.0000	0.9990

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Binary toluene–butanol mixtures (100 g) of known composition in 300 mL glass stoppered bottles were titrated with distilled water until a second phase appeared and persisted on prolonged vigorous shaking.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/ °C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.019	0.000	0.074	0.000
		0.488	0.000	0.797	0.000
		0.524	0.034	0.778	0.063
		0.527	0.047	0.765	0.085
		0.548	0.110	0.714	0.178
		0.534	0.190	0.638	0.282
		0.506	0.271	0.564	0.376
		0.462	0.372	0.479	0.479
		0.398	0.481	0.388	0.583
		0.322	0.603	0.295	0.688
		0.225	0.725	0.198	0.792
		0.118	0.858	0.099	0.896
		0.060	0.928	0.049	0.948
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/ °C	T/K (compiler)	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.341	0.570	0.007	0.000	0.318	0.661	0.028	0.000
		0.455	0.382	0.012	0.000	0.469	0.490	0.048	0.000
		0.542	0.090	0.016	0.000	0.729	0.151	0.063	0.000
		0.488	0.000	0.019	0.000	0.797	0.000	0.074	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by the addition of anhydrous potassium carbonate, distilled; purity better than 99.6 mole % by glc.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) 1-Heptene; C_7H_{14}; [592-76-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, B. C. Bricknell, J. D. Sewry, and S. E. Radloff, J. Chem. Eng. Data **39**, 320–3 (1994).

Variables:

T/K=298

Compiled by:

A. Skrzecz

9.5. 1-Butanol + Water + 1-Heptene

Experimental Data

Compositions along the saturation curve

t/ °C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	1.000	0.000	1.000
		0.142	0.834	0.113	0.882
		0.259	0.683	0.220	0.768
		0.354	0.546	0.321	0.657
		0.432	0.426	0.419	0.547
		0.491	0.317	0.513	0.439
		0.527	0.231	0.591	0.343
		0.545	0.150	0.666	0.243
		0.549	0.091	0.725	0.159
		0.532	0.038	0.775	0.073
		0.485	0.000	0.795	0.000
		0.019	0.000	0.074	0.000
		0.010	0.001	0.040	0.005

Compositions of coexisting phases

		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
t/ °C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
25.0	298.2	0.543	0.168	0.015	0.000	0.650	0.266	0.059	0.000
		0.396	0.487	0.009	0.001	0.370	0.603	0.036	0.005
		0.190	0.780	0.004	0.000	0.154	0.840	0.016	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods have been described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) Aldrich; distilled; purity>99.8 mole % by glc, ρ=0.692 65 gc m^{-3}.
(3) not specified.

Estimated Error:

Not reported.

References:

[1]T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:

T/K=298

Compiled by:

A. Skrzecz

9.6. 1-Butanol + Water + Heptane

Experimental Data

Compositions along the saturation curve

t/ °C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.495	0.000	0.801	0.000
		0.545	0.044	0.774	0.084
		0.525	0.209	0.602	0.324
		0.492	0.311	0.512	0.438
		0.369	0.534	0.331	0.648
		0.148	0.836	0.115	0.882
		0.014	0.000	0.055	0.000

Compositions of coexisting phases

		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
t/ °C (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
25	298.2	0.525	0.131	0.011	0.000	0.668	0.225	0.044	0.000
		0.409	0.491	0.008	0.000	0.373	0.605	0.032	0.000
		0.129	0.865	0.005	0.000	0.099	0.900	0.020	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) Aldrich, 99 mole %; dried with magnesium metal activated with iodine, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1]S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).

Components:	Original Measurements:
(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3] (2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3] (3) Water; H_2O; [7732-18-5]	T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053–60 (1989).
Variables: T/K=298	**Compiled by:** A. Skrzecz

9.7. 1-Butanol + Water + *p*-Xylene

Experimental Data

Compositions along the saturation curve

t/ °C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.998	0.000	0.9997
		0.070	0.915	0.051	0.947
		0.133	0.837	0.099	0.895
		0.248	0.691	0.198	0.790
		0.341	0.557	0.293	0.686
		0.415	0.434	0.387	0.579
		0.474	0.330	0.477	0.475
		0.514	0.239	0.561	0.374
		0.534	0.093	0.705	0.176
		0.539	0.070	0.734	0.137
		0.491	0.003	0.794	0.007
		0.488	0.000	0.797	0.000
		0.020	0.000	0.077	0.000

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/ °C (compiler)	T/K	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.488	0.000	0.020	0.000	0.797	0.000	0.077	0.000
		0.542	0.140	0.015	0.000	0.661	0.245	0.059	0.000
		0.399	0.463	0.010	0.000	0.364	0.605	0.040	0.000
		0.170	0.788	0.005	0.000	0.130	0.862	0.020	0.000
		0.000	0.998	0.000	0.000	0.000	0.9997	0.000	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. A binary mixture of known composition was titrated with the third component until cloudiness was observed. Tie line compositions were related to the coexistence curve; water was determined by the Karl Fischer titration. The methods were described in Ref. 1.

Source and Purity of Materials:

(1) source not specified; used as received.
(2) source not specified; recrystallized three times.
(3) not specified.

Estimated Error:

comp. <0.005 mole fraction (estimated authors' precision on binodal curve), <0.01 mole fraction (estimated authors' precision of tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

Components:	Original Measurements:
(1) 1-Butanol (*n*-butanol, butyl alcohol, *n*-butyl alcohol); $C_4H_{10}O$; [71-36-3] (2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12}; [108-67-8] (3) Water; H_2O; [7732-18-5]	T. M. Letcher and P. M. Siswana, Fluid Phase Equilib, **74**, 203–17 (1992).
Variables: T/K=298	**Compiled by:** A. Skrzecz

9.8. 1-Butanol + Water + Mesitylene

Experimental Data

Compositions along the saturation curve

t/ °C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.019	0.000	0.074	0.000
		0.488	0.000	0.797	0.000
		0.493	0.002	0.796	0.005
		0.530	0.034	0.767	0.080
		0.546	0.083	0.708	0.175
		0.541	0.143	0.637	0.273
		0.496	0.306	0.477	0.477
		0.436	0.404	0.386	0.580
		0.365	0.525	0.294	0.685
		0.269	0.664	0.198	0.791
		0.146	0.814	0.099	0.894
		0.077	0.902	0.050	0.947
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/ °C	T/K (compiler)	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.361	0.530	0.007	0.000	0.290	0.689	0.028	0.000
		0.491	0.315	0.010	0.000	0.468	0.487	0.040	0.000
		0.545	0.070	0.015	0.000	0.725	0.151	0.059	0.000
		0.488	0.000	0.019	0.000	0.797	0.000	0.074	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by the addition of anhydrous potassium carbonate, distilled; purity better than 99.6 mole % by glc.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:
estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:
[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

10. 2-Butanol+Water

Components:
(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2-butanol); C_4H_{10} ; [78-92-2]
(2) Butane (*n*-butane); C_4H_{10} ; [106-97-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
M. Radosz, Fluid Phase Equilib. **29**, 515–23 (1986).

Variables:
T/K=393–449

Compiled By:
A. Skrzecz

10.1. 2-Butanol + Water + Butane

Experimental Data

Compositions of coexisting phases

			x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C (compiler)	T/K	p/MPa	hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
119.7	392.9	0.50	—	—	—	—	—	—	—	—[a]
119.7	392.9	0.61	0.0580	0.0004	0.2444	0.0083	0.202	0.001	0.565	0.015
120.2	393.4	2.03	0.0169	0.0003	0.3483	0.4813	0.066	0.001	0.454	0.492
119.7	392.9	2.05	—	—	—	—	—	—	—	—[b]
174.9	448.1	3.03	—	—	—	—	—	—	—	—[a]
174.9	448.1	3.45	0.0473	0.0018	0.3250	0.0906	0.169	0.005	0.604	0.132
175.4	448.6	3.45	0.0106	0.0006	0.0944	0.6737	0.042	0.002	0.139	0.778
176.1	449.3	3.45	0.0150	0.0006	0.1201	0.6440	0.059	0.002	0.176	0.740
174.7	447.9	4.48	0.0258	0.0010	0.3506	0.3720	0.098	0.003	0.494	0.411
175.4	448.6	4.48	0.0108	0.0006	0.0919	0.7487	0.043	0.002	0.128	0.818
175.9	449.1	4.48	0.0137	0.0006	0.1112	0.7207	0.054	0.002	0.155	0.788
174.9	448.1	4.96	—	—	—	—	—	—	—	—[b]

[a] Lower pressure end point for liquid–liquid–vapor equilibrium.
[b] Upper pressure end point for liquid–vapor equilibrium.

Auxiliary Information

Method/Apparatus/Procedure:

A variable-volume circulation apparatus with two circulation pumps was used for investigation of three-phase (liquid–liquid–vapor) equilibria. A batch windowed cell (mixing and separating vessel) allows on visual observation of phase transition. Analysis were made by an on-line gas chromatograph. The experimental equipment was reported in Ref. 1.

Source and Purity of Materials:

(1) Fischer Scientific Co., 99 + % purity; used as received.
(2) Mathenson Gas Products, ‘‘Instrument Purity’’ 99.5 + % purity; used as received.
(3) not specified.

Estimated Error:
Not reported.

References:
[1] M. Radosz, Ber. Bunsen-Ges. Phys. Chem. **88**, 859 (1984).

Components:

(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2-butanol); $C_4H_{10}O$; [78-92-2]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1997.05)

10.2. 2-Butanol + Water + Benzene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-butanol–benzene–water is given in Table 78.

TABLE 78. Summary of experimental data for the system 2-butanol–benzene–water

Author(s)	T/K	Type of data[a]	Ref.
Davis and Evans, 1960	303	sat. (17), eq. (10)	1
Letcher *et al.*, 1990	298	sat. (13), eq.(4)	2

[a]Number of experimental points in parentheses.

The ternary system 2-butanol–benzene–water forms a miscibility gap of type 2. Two binary systems, benzene–water and 2-butanol–water, form miscibility gaps. These systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. These recommended values of mutual solubility at 303 K are $x_2'=0.996\,40$, $x_2''=0.000\,418$ for the benzene–water system, and $x_1'=0.318$, $x_1''=0.0491$ for the 2-butanol–water system. Both types of data reported by Davis and Evans[1] are consistent with one another as a binodal curve. The data of Letcher *et al.*[2] were reported in graphical form only and therefore are not compiled. The maximum alcohol concentration on the binodal curve at 298 K, $x_1=0.50$, Ref. 2, is consistent with the results of Davis and Evans at 303 K,[1] $x_1=0.499$. The experimental tie lines at 303.2 K[1] are shown in Fig. 42 together with the experimental points along the saturation curve.

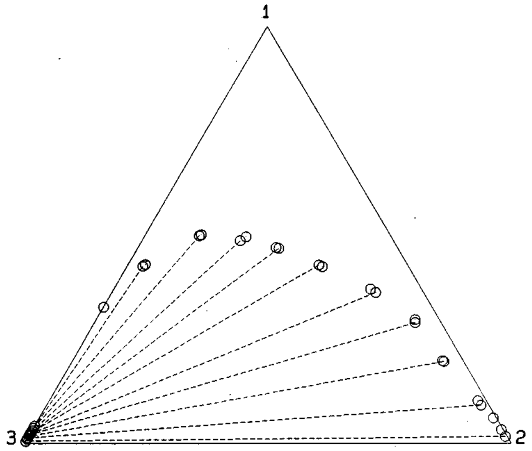

FIG. 42. Phase diagram of the system 2-butanol (1)—benzene (2)—water (3) at 303.2 K. ○—experimental results of Ref. 1, dashed lines—experimental tie lines, Ref. 1.

References:

[1]J. R. Davis and L. R. Evans, J. Chem. Eng. Data **5**, 401 (1960).
[2]T. M. Letcher, J. Sewry, and S. Radloff, S. Afr. J. Chem. **43**, 56 (1990).
[3]D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).
[4]A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2-butanol); $C_4H_{10}O$; [78-92-2]
(2) Benzene; C_6H_6 ; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements

J. R. Davis and L. R. Evans, J. Chem. Eng. Data **5**, 401–2 (1960)

Variables:

T/K=303

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
30.0	303.15	0.0326	0.9627	0.0311	0.9678
		0.0606	0.9321	0.0580	0.9403
		0.1024	0.8793	0.0991	0.8966
		0.1977	0.7591	0.1961	0.7935
		0.2954	0.6537	0.2964	0.6912
		0.3685	0.5254	0.3887	0.5841
		0.4221	0.3999	0.4760	0.4752
		0.4682	0.2825	0.5665	0.3602
		0.4939	0.2083	0.6285	0.2794
		0.4989	0.1145	0.6992	0.1691
		0.4275	0.0348	0.7187	0.0616
		0.0315	0.0002	0.1180	0.0006
		0.0202	0.0001	0.0783	0.0006
		0.0102	0.0002	0.0407	0.0007
		0.0046	0.0003	0.0186	0.0012
		0.3254	0.0000	0.6650	0.0000
		0.0418	0.0000	0.1523	0.0000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
30.0	303.15	0.0162	0.9791	0.0054	0.0002	0.0154	0.9835	0.0218	0.0008
		0.0912	0.8918	0.0134	0.0002	0.0881	0.9079	0.0530	0.0008
		0.1959	0.7629	0.0177	0.0001	0.1940	0.7961	0.0690	0.0006
		0.2882	0.6578	0.0202	0.0001	0.2898	0.6970	0.0781	0.0006
		0.3601	0.5402	0.0221	0.0001	0.3776	0.5970	0.0849	0.0004
		0.4260	0.3910	0.0257	0.0001	0.4827	0.4669	0.0978	0.0005
		0.4666	0.2891	0.0263	0.0001	0.5617	0.3668	0.0999	0.0005
		0.4847	0.2010	0.0271	0.0001	0.6271	0.2741	0.1028	0.0004
		0.4968	0.1114	0.0307	0.0001	0.7003	0.1655	0.1154	0.0005
		0.4231	0.0318	0.0365	0.0001	0.7182	0.0569	0.1347	0.0003

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities and tie lines were measured in 25 mL glass-stoppered flasks, mounted in an air-shaker and immersed in a constant temperature bath by titration of weighed mixtures to the appearance of a permanent second phase. The third component was added by hypodermic syringe. Drops were 2–3 mg. The experimental results were accepted when the loss of vapors was smaller than 17 mg (about 0.2% of the total volume). Refractive indexes of the saturation solutions were measured at 30 °C by an Abbe 3 L refractometer and plotted as a concentration function for each component. The tie lines were determined by adding alcohol to binary benzene–water mixtures. After separation, refraction indexes were measured for each phase and the concentrations were read from prepared plots. The sum of calculated concentration was always 1.000 ±0.001 of mass fraction.

Source and Purity of Materials:

(1) Matheson Co.; dried over Na, distilled; $n(20\ °C)=1.3974$, $d(20\ °C)=0.8050$.
(2) source not specified; dried over Na, distilled; $n(20\ °C)=1.5001$, $d(20\ °C)=0.8795$.
(3) de-ionized, distilled from $KMnO_4$; $n(20\ °C)=1.3343$, $d(20\ °C)=0.9979$.

Estimated Errors:

bath temp. ±0.05 °C (solubility), ±0.02 °C (tie line).

Components:	**Evaluated by:**
(1) 2-Butanol (sec-butanol; sec-butyl alcohol; (RS)-2-butanol; dl-2-butanol; DL-2-butanol); $C_4H_{10}O$; [78-92-2] (2) Cyclohexane; C_6H_{12} ; [110-82-7] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1995.09)

10.3. 2-Butanol + Water + Cyclohexane

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-butanol–cyclohexane–water is given in Table 79.

TABLE 79. Summary of experimental data for the system 2-butanol–cyclohexane–water

Author(s)	T/K	Type of data[a]	Ref.
Plackov and Stern, 1990	298	sat. (13), eq. (8)	1
Letcher *et al.*, 1991	298	sat. (16), eq. (5)	2

[a]Number of experimental points in parentheses.

Saturation curve

The ternary system 2-butanol–cyclohexane–water forms a miscibility gap of type 2. The system was studied by titration method at 298.2 K by both investigators. Two binary systems cyclohexane–water and 2-butanol–water form miscibility gaps. The data for these binary systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. The recommended values of mutual solubility at 298 K are: for cyclohexane–water system $x_2''=1.2\cdot 10^{-5}$ and $x_3'=3.7\cdot 10^{-4}$, Ref. 3, and for 2-butanol–water system $x_1'=0.322$ and $x_1''=0.051$, Ref. 4. Letcher *et al.*[2] reported ternary data and mutual solubility for binary systems. The end points of saturation curve were reported to be $x_2'=0.999$ and pure water. This is inconsistent with the recommended values but within the accuracy of experimental measurements (0.001 mole fraction) stated by the authors. Binary solubility data of the 2-butanol–water system reported in Ref. 2 as $x_1'=0.312$ and $x_1''=0.051$ are consistent with the ''best values'' reported in the critical evaluation, Ref. 3. Plackov and Stern[1] reported only solubility of 2-butanol in water, $x_1''=0.0544$. This result is also consistent with recommended data. These experimental data are consistent with one another.

Compositions of the water-rich phase of the ternary system, Refs. 1 and 2, were reported as binary 2-butanol–water mixtures. The analytical methods could not detect cyclohexane. Therefore the water-rich branch could not be evaluated. Phase equilibrium data were used to construct the saturation curve for the organic-rich phase. Data for 298.2 K were described by the equation:

$$x_1=0.683\ 11+0.066\ 20\ \ln(x_2)-0.341\ 40x_2-0.349\ 78x_2^2.$$

The model describes the region $0.01<x_2<0.96$. The parameters were calculated by the least-squares method. The standard error of estimate was 0.0061. The points on the saturation curve calculated by this equation for selected concentrations of cyclohexane in the mixture are presented in Table 80 and in Fig. 43 as a calculated binodal curve (solid line).

TABLE 80. Calculated compositions along the saturation curve at 298.2 K

x_1	x_2	x_1	x_2
0.322	0.000 Ref. 4	0.3677	0.5200
0.3748	0.0100	0.3560	0.5400
0.4172	0.0200	0.3438	0.5600
0.4558	0.0400	0.3314	0.5800
0.4751	0.0600	0.3185	0.6000
0.4863	0.0800	0.3053	0.6200
0.4930	0.1000	0.2918	0.6400
0.4967	0.1200	0.2779	0.6600
0.4983	0.1400	0.2637	0.6800
0.4982	0.1600	0.2491	0.7000
0.4968	0.1800	0.2342	0.7200
0.4943	0.2000	0.2190	0.7400
0.4908	0.2200	0.2034	0.7600
0.4865	0.2400	0.1876	0.7800
0.4815	0.2600	0.1714	0.8000
0.4758	0.2800	0.1548	0.8200
0.4695	0.3000	0.1380	0.8400
0.4626	0.3200	0.1208	0.8600
0.4552	0.3400	0.1033	0.8800
0.4472	0.3600	0.0855	0.9000
0.4388	0.3800	0.0674	0.9200
0.4299	0.4000	0.0490	0.9400
0.4206	0.4200	0.0303	0.9600
0.4108	0.4400	0.0000	0.99963 Ref. 3
0.4006	0.4600	0.0000	0.000012 Ref. 3
0.3901	0.4800	0.051	0.0000 Ref. 4
0.3791	0.5000		

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 2-butanol–cyclohexane–water were reported in two references at 298.2 K using similar experimental procedures. First equilibrium was reached, then the phases were separated and the composition of each phase was determined. Compositions of water-rich phase in equilibrium were reported as binary 2-butanol–water mixtures; the analytical methods could not detect cyclohexane. The tie lines cover the whole area of the miscibility gap and are consistent within each data set. Distribution of 2-butanol differs between data sets with Letcher *et al.*[2] reporting lower concentrations of alcohol in the water-rich phase than Plackov and Stern.[1] Both data sets are treated as tentative. All experimental data points at 298.2 K are reported in Fig. 43.

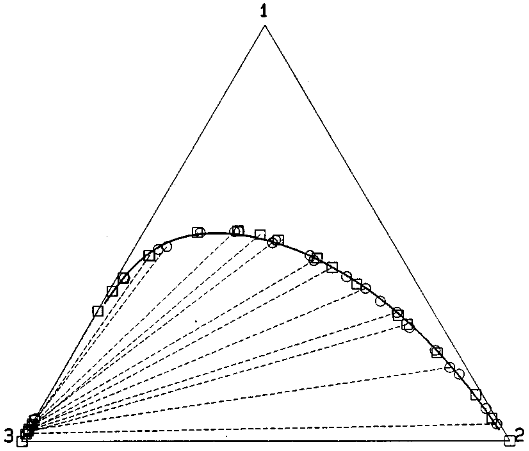

FIG. 43. Phase diagram of the system 2-butanol (1)—cyclohexane (2)—water (3) at 298.2 K. Solid line—calculated binodal curve, ○—experimental results of Ref. 1, □—experimental results of Ref. 2, dashed lines—experimental tie lines, Refs. 1 and 2.

References:

[1]D. Plackov and I. Stern, Fluid Phase Equilib **57**, 327 (1990).

[2]T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118 (1991).

[3]D. G. Shaw, ed., *Solubility Data Series,* Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[4]A. F. M. Barton, ed., *Solubility Data Series,* Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 2-Butanol (sec-butanol, sec-butyl alcohol (RS)-2-butanol, dl-2-butanol, DL-2-butanol); $C_4H_{10}O$; [78-92-2]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. Plackov and I. Stern, Fluid Phase Equilib. **57**, 327–40 (1990).

Variables:

T/K=298

Compiled By:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.00	298.15	0.0779	0.9118	0.0698	0.9279
		0.1610	0.8160	0.1473	0.8476
		0.2181	0.7386	0.2044	0.7858
		0.2727	0.6585	0.2629	0.7209
		0.3354	0.5677	0.3342	0.6423
		0.3943	0.4688	0.4108	0.5545
		0.4450	0.3680	0.4899	0.4600
		0.4815	0.2793	0.5620	0.3701
		0.5025	0.1943	0.6306	0.2769
		0.4998	0.1160	0.6895	0.1817
		0.4591	0.0500	0.7228	0.0894
		0.3916	0.0152	0.7081	0.0312
		0.0544	0.0000	0.1914	0.0000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.00	298.15	0.041	0.952	0.018	0.000	0.036	0.962	0.070	0.000
		0.177	0.789	0.024	0.000	0.164	0.829	0.092	0.000
		0.309	0.615	0.026	0.000	0.301	0.681	0.099	0.000
		0.366	0.522	0.027	0.000	0.371	0.601	0.102	0.000
		0.433	0.382	0.036	0.000	0.475	0.476	0.133	0.000
		0.475	0.276	0.038	0.000	0.559	0.369	0.140	0.000
		0.502	0.185	0.039	0.000	0.637	0.266	0.143	0.000
		0.466	0.064	0.042	0.000	0.714	0.111	0.153	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, as reported in Ref. 1, was used to determine the solubility curve. Mixtures of known composition, mixed by means of a magnetic stirrer and placed in the thermostated double-wall Erlenmayer flask, were titrated with the less soluble component until the appearance of turbidity. The analytical method was used to determine liquid–liquid equilibria. The mixture was shaken for at least 20 min. Equilibration took place in a thermostated double-walled separatory funnel of 250 mL over 2 h. The refractive index and density of both phases were measured. The composition was calculated numerically from the calibration data by polynomial regression analysis. The third order polynomials were used. Each experiment was repeated three times.

Source and Purity of Materials:

(1) Merck, analytical grade; used as received; $n=1.3943$, $\rho(25\ °C)=802.5\ kg\ m^{-3}$, b.p.=99.3 °C.
(2) Kemika (Zagreb), analytical grade; used as received; $n=1.4232$, $\rho(25\ °C)=773.6\ kg\ m^{-3}$, b.p.=80.0 °C.
(3) double distilled in the presence of $KMnO_4$.

Estimated Error:

temp ±0.02 °C; composition <±0.05% (by mass) relative error.

References:

[1] E. R. Washburn, C. L. Graham, G. B. Arnold, and L. F. Transuel, J. Am. Chem. Soc. **62**, 1454 (1940).

Components:

(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2-butanol); $C_4H_{10}O$; [78-92-2]
(2) Cyclohexane; C_6H_{12} ; [110-82-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, P. Siswana, and S. E. Radloff, S. Afr. J. Chem. **44**, 118–21 (1991).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.051	0.000	0.181	0.000
		0.312	0.000	0.651	0.000
		0.360	0.006	0.691	0.013
		0.391	0.013	0.710	0.027
		0.445	0.038	0.725	0.070
		0.500	0.110	0.695	0.174
		0.504	0.191	0.634	0.273
		0.482	0.284	0.560	0.374
		0.438	0.386	0.477	0.477
		0.377	0.498	0.388	0.581
		0.302	0.621	0.294	0.687
		0.212	0.746	0.198	0.792
		0.111	0.875	0.100	0.897
		0.055	0.935	0.049	0.949
		0.000	0.999	0.0000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C (compiler)	T/K	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.312	0.000	0.051	0.000	0.651	0.000	0.181	0.000
		0.445	0.040	0.042	0.000	0.723	0.074	0.153	0.000
		0.495	0.241	0.030	0.000	0.594	0.329	0.113	0.000
		0.416	0.428	0.025	0.000	0.443	0.517	0.095	0.000
		0.280	0.650	0.018	0.000	0.271	0.713	0.070	0.000

Auxiliary Information

Method/Appratus/Procedure:

The points on the binodal curve were determined by the titration method, as described in Ref. 1. The formation of a cloudy mixture was observed visually on shaking after addition of a known mass of the third component; syringes were precisely weighed. Tie line compositions were determined by the refractive index method, Ref. 2, and a complementary method using the Karl Fischer titration, Ref. 3. Measurements were made at pressure of 94.7 kPa.

Source and Purity of Materials

(1) Merck; AR grade; dried by addition of anhydrous K_2CO_3, distilled; purity >99.9 mole % by glc.
(2) BDH; Gold label grade; used as received; purity >99.9 mole % by glc.
(3) not specified.

Estimated Error:

composition ±0.005 mole fraction (binodal curve), ±0.01 mole fraction (tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs, and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

Components:	**Evaluated by:**
(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol); $C_4H_{10}O$; [78-92-2] (2) Toluene (methylbenzene); C_7H_8; [108-88-3] (3) Water; H_2O; [7732-18-5]	A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.06)

10.4. 2-Butanol + Water + Toluene

Critical Evaluation:

A survey of reported compositions along the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 2-butanol–toluene–water is given in Table 81.

TABLE 81. Summary of experimental data for the system 2-butanol–toluene–water

Author(s)	T/K	Type of data[a]	Ref.
Evans and Lin, 1968	298	sol. (21), eq. (5)	1
Letcher and Siswana, 1992	298	sol. (15), eq. (4)	2

[a] Number of experimental points in parentheses.

Saturation curve

The system 2-butanol–toluene–water forms a miscibility gap of type 2. Two binary systems, 2-butanol–water and toluene–water are partially miscible. The data of these systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. The recommended values of mutual solubility of toluene–water system at 298.2 K are: $x_2'=0.9972$ and $x_2''=0.000\,104$ (Ref. 3). The mutual solubility of 2-butanol–water system at 298.2 K calculated on the basis of Ref. 4 are: $x_1'=0.322$ and $x_1''=0.0510$. Letcher and Siswana[2] report at 298.2 K mutual solubility of the binary systems toluene–water and 2-butanol–water as $x_2'=0.999$, $x_2''=0.000$ and $x_1'=0.312$, $x_1''=0.051$, respectively. These binary data are consistent with recommended data since they are within the accuracy estimated by the authors (0.01 mole fraction). The experimental data on saturation curve were reported in Refs. 1 and 2 at the same temperature and are consistent with one another. Data presented by Evans and Lin[1] show the miscibility gap slightly to be smaller (of about 0.02–0.03 mole fraction of water) than found by Letcher and Siswana,[2] especially in the region of $0.26<x_2<0.75$. The maximum 2-butanol concentration observed on the organic-rich branch of the saturation curve at 298 K is $x_1=0.489\pm0.005$. The data for the organic-rich phase of the saturation curve,[1,2] (points reported as phases in equilibrium were included) were used to construct the equation:

$$x_1=0.618\,84+0.053\,26\ln(x_2)-0.183\,05x_2-0.452\,04x_2^2.$$

The model applies to the region $0.004<x_2<0.94$. The parameters were calculated by the least-squares method and the standard error of estimate was 0.0083. There was an error (presumably a typographic) in Ref. 2 at the point $x_1=0.120$ $x_2=0.885$ on saturation curve (the sum of compositions was greater than 1.0) and this experimental point was rejected. Selected points on the saturation curve, calculated by the above equation together with the ''best'' values of Refs. 3 and 4 are presented in Table 82 and as solid line in Fig. 44. The water-rich branch of saturation curve contains small amount of toluene ($x_2<0.0001$) and toluene concentration was not reported in either paper. These experimental points were not described by any model.

TABLE 82. Calculated compositions along the saturation curve at 298.2 k (organic-rich phase)

x_1	x_2	x_1	x_2
0.312	0.0000 Ref. 4	0.3774	0.5000
0.3717	0.0100	0.3666	0.5200
0.4066	0.0200	0.3554	0.5400
0.4394	0.0400	0.3437	0.5600
0.4564	0.0600	0.3316	0.5800
0.4668	0.0800	0.3191	0.6000
0.4734	0.1000	0.3061	0.6200
0.4774	0.1200	0.2928	0.6400
0.4796	0.1400	0.2790	0.6600
0.4804	0.1600	0.2648	0.6800
0.4799	0.1800	0.2502	0.7000
0.4784	0.2000	0.2198	0.7400
0.4761	0.2200	0.2198	0.7400
0.4729	0.2400	0.2040	0.7600
0.4689	0.2600	0.1878	0.7800
0.4644	0.2800	0.1712	0.8000
0.4591	0.3000	0.1542	0.8200
0.4533	0.3200	0.1368	0.8400
0.4469	0.3400	0.1191	0.8600
0.4399	0.3600	0.1009	0.8800
0.4325	0.3800	0.0823	0.9000
0.4245	0.4000	0.0634	0.9200
0.4160	0.4200	0.0441	0.9400
0.4071	0.4400	0.0000	0.9972 Ref. 3
0.3976	0.4600	0.0000	0.000 104 Ref. 3
0.3877	0.4800	0.1510	0.0000 Ref. 4

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 2-butanol–toluene–water were reported in both references at 298.2 K and cover the whole range of the miscibility gap. The compositions of phases in equilibrium reported in Refs. 1 and 2 are consistent with one another. Both data sets are considered tentative. All experimental tie lines are presented in Fig. 44 together with experimental points forming the solubility curve.

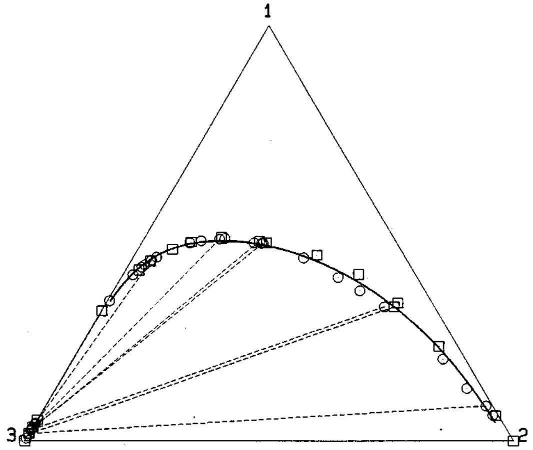

FIG. 44. Phase diagram of the system 2-butanol (1)—toluene (2)—water (3) at 298.2 K. Solid line—recommended saturation curve, ○—experimental data, Ref. 1, ☐—experimental data, Ref. 2, dashed lines—experimental tie lines, Refs. 1 and 2.

Referencs:

[1] L. R. Evans and J. S. Lin, J. Chem. Eng. Data **13,** 14 (1968).

[2] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[4] A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol); $C_4H_{10}O$; [78-92-2]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. R. Evans and J.-S. Lin, J. Chem. Eng. Data **13**, 14–6 (1968).

Variables:

T/K=295

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25.0	298.15	0.0617	0.9263	0.0507	0.9469
		0.1268	0.8407	0.1075	0.8858
		0.1970	0.7571	0.1714	0.8189
		0.3221	0.5756	0.3032	0.6734
		0.3606	0.5057	0.3529	0.6153
		0.3928	0.4453	0.3985	0.5616
		0.4395	0.3511	0.4742	0.4709
		0.4744	0.2468	0.5588	0.3614
		0.4757	0.2307	0.5705	0.3439
		0.4862	0.1656	0.6260	0.2650
		0.4758	0.0982	0.6784	0.1740
		0.4412	0.0472	0.7068	0.0940
		0.4226	0.0319	0.7104	0.0667
		0.4170	0.0289	0.7097	0.0611
		0.3985	0.0197	0.7061	0.0434
		0.3364	0.0036	0.6710	0.0090
		0.0424	0.0000	0.1541	0.0000
		0.0276	0.0000	0.1044	0.0000
		0.0179	0.0000	0.0696	0.0000
		0.0062	0.0000	0.0251	0.0000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25.0	298.15	0.0845	0.9006	0.0166	0.0000	0.0700	0.9270	0.0650	0.0000
		0.3222	0.5747	0.0254	0.0000	0.3035	0.6729	0.0970	0.0000
		0.4748	0.2499	0.0304	0.0000	0.5570	0.3645	0.1141	0.0001
		0.4848	0.1551	0.0331	0.0000	0.6336	0.2520	0.1235	0.0000
		0.4340	0.0401	0.0398	0.0000	0.7095	0.0815	0.1457	0.0000

Auxiliary Information

Method/Apparatus/Procedure:

Solubilities and tie lines were measured in 50 mL glass-stoppered flasks, mounted in a motor-driven shaker and immersed in a constant temperature bath. To obtain solubilities, the weighed mixtures were titrated to the appearance of a permanent second phase. The third component was added by hypodermic syringe in drops of about 4 mg. Equilibrium was reached when the second phase persisted after 1 h shaking in the bath. The evaporation loss was about 20 mg (0.1%–0.2% of the total solution). Refractive indexes of the saturated solutions were measured at 20 °C with a Bausch and Lomb 3 L refractometer and plotted as a concentration function for each component. The tie lines were determined by shaking three-component mixtures of known composition in a constant temperature bath for 6 h. After separation, refractive indexes were measured for each phase and the concentrations were read from prepared plots. The sum of calculated concentrations was always 1.000±0.001 when expressed as mass fraction. The procedure was the same as in Ref. 1.

Source and Purity of Materials:

(1) Eastman Kodak. Co.; treated with $MgSO_4$, dried over Na, distilled; $n(20\ °C)=1.3973$, $d(20\ °C)=0.8059$.
(2) J. T. Barker Chemical Co.; dried over Na, distilled; $n(20\ °C)=1.4963$, $d(20\ °C)=0.8667$.
(3) de-ionized, distilled from $KMnO_4$; $n(20\ °C)=1.3324$, $d(20\ °C)=0.9983$.

Estimated Error:

bath temp. ±0.05 °C (solubility).

References:

[1] J. R. Davis and L. R. Evans, J. Chem. Eng. Data **5**, 401 (1960).

Components:

(1) 2- Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2-butanol);$C_4H_{10}O$;[78-92-2]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
25.0	298.2	0.000	0.000	0.000	0.000
		0.051	0.000	0.181	0.000
		0.312	0.000	0.651	0.000
		0.410	0.027	0.706	0.058
		0.432	0.039	0.709	0.080
		0.460	0.070	0.696	0.132
		0.478	0.100	0.678	0.176
		0.489	0.157	0.635	0.253
		0.476	0.256	0.554	0.370
		0.446	0.375	0.467	0.488
		0.400	0.483	0.389	0.584
		0.331	0.598	0.303	0.681
		0.227	0.734	0.198	0.794
		0.061	0.933	0.050	0.949

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.322	0.595	0.018	0.000	0.298	0.684	0.070	0.000
		0.480	0.240	0.033	0.000	0.567	0.352	0.123	0.000
		0.312	0.000	0.051	0.000	0.651	0.000	0.181	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by the addition of anhydrous potassium carbonate, distilled; purity better than 99.6 mole % by glc.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and E. W Comings, Ind. Eng. Chem **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21,** 1053 (1989).

Components:

(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2 butanol); $C_4H_{10}O$; [78-92-2]
(2) 1-Heptene; C_7H_{14}; [592-76-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, B. C. Bricknell, J. D. Sewry, and S. E. Radloff, J. Chem. Eng. Data **39**, 320–3 (1994).

Variables:

T/K=298

Compiled by:

A. Skrzecz

10.5. 2-Butanol + Water + 1-Heptene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	1.000	0.000	1.000
		0.142	0.828	0.114	0.880
		0.255	0.683	0.217	0.770
		0.391	0.489	0.366	0.607
		0.430	0.426	0.418	0.548
		0.485	0.323	0.505	0.446
		0.520	0.231	0.587	0.345
		0.521	0.147	0.654	0.245
		0.498	0.082	0.703	0.153
		0.452	0.037	0.723	0.078
		0.322	0.000	0.661	0.000
		0.054	0.000	0.190	0.000
		0.023	0.001	0.088	0.005
		0.000	0.000	0.000	0.000

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C	T/K (compiler)	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.527	0.183	0.042	0.000	0.627	0.289	0.153	0.000
		0.400	0.478	0.027	0.001	0.376	0.596	0.102	0.005
		0.170	0.785	0.011	0.000	0.139	0.852	0.044	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The experimental methods have been described in Ref. 1. No more details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) Aldrich; distilled; purity >99.8 mole % by glc, $\rho = 0.692\ 65$ g cm^{-3}.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203 (1992).

Components:

(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2-butanol); $C_4H_{10}O$; [78-92-2]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:

T/K=298

Compiled by:

A. Skrzecz

10.6. 2-Butanol + Water + Heptane

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.348	0.000	0.687	0.000
		0.443	0.028	0.727	0.062
		0.513	0.143	0.649	0.245
		0.484	0.305	0.511	0.435
		0.367	0.528	0.332	0.645
		0.159	0.825	0.124	0.873
		0.057	0.000	0.199	0.000

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C (compiler)	T/K	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25	298.2	0.453	0.374	0.030	0.000	0.453	0.505	0.113	0.000
		0.224	0.736	0.025	0.000	0.182	0.810	0.095	0.000
		0.127	0.862	0.017	0.000	0.098	0.900	0.066	0.000

Auxiliatry Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) Aldrich, Gold label, 99.5 mole %; dried with anhydrous potassium carbonate, filtrated, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1] S. W. Brigg, and E. W. Comings, Ind. Eng. Chem. **35**, 441 (1993).

Components:	**Original Measurements:**
(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2-butanol); $C_4H_{10}O$; [78-92-2] (2) *p*-Xylene (1,4-dimethylbenzene, 1,4-xylene); C_8H_{10}; [106-42-3] (3) Water; H_2O; [7732-18-5]	T. M. Letcher, P. M. Siswana, P. van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053–60 (1989).
Variables: T/K=298	**Compiled by:** A. Skrzecz

10.7. 2-Butanol + Water + *p*-Xylene

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.998	0.000	0.9997
		0.070	0.916	0.051	0.947
		0.134	0.842	0.100	0.896
		0.248	0.693	0.198	0.791
		0.341	0.555	0.294	0.685
		0.412	0.431	0.386	0.578
		0.462	0.322	0.474	0.473
		0.494	0.231	0.554	0.371
		0.503	0.150	0.627	0.268
		0.486	0.085	0.683	0.171
		0.414	0.021	0.712	0.052
		0.360	0.006	0.689	0.016
		0.330	0.002	0.666	0.006
		0.322	0.000	0.661	0.000
		0.051	0.000	0.181	0.000

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K	organic-rich phase		water-rich phase		organic-rich phase		water-rich phase	
25.0	298.2	0.322	0.000	0.051	0.000	0.661	0.000	0.181	0.000
		0.490	0.230	0.040	0.000	0.552	0.371	0.146	0.000
		0.385	0.480	0.026	0.000	0.348	0.622	0.099	0.000
		0.130	0.843	0.015	0.000	0.097	0.898	0.059	0.000
		0.000	0.998	0.000	0.000	0.000	0.9997	0.000	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to determine binodal curve. A binary mixture of known composition was titrated with the third component until cloudiness was observed. Tie line compositions were related to the coexistence curve; water was determined by the Karl Fischer titration. The methods were described in Ref. 1.

Source and Purity of Materials:

(1) source not specified; used as recieved.
(2) source not specified; recrystallized three times.
(3) not specified.

Estimated Error:

comp. <0.005 mole fraction (estimated authors' precision on binodal curve), <0.01 mole fraction (estimated authors' precision of tie lines).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037 (1986).

Components:

(1) 2-Butanol (sec-butanol, sec-butyl alcohol, (RS)-2-butanol, dl-2-butanol, DL-2-butanol); $C_4H_{10}O$; [78-92-2]
(2) Mesitylene (1,3,5-trimethylbenzene); C_9H_{12}; [108-67-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher and P. M. Siswana, Fluid Phase Equilib. **74**, 203–17 (1992).

Variables:

T/K=298

Compiled by:

A. Skrzecz

10.8. 2-Butanol + Water + Mesitylene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25.0	298.2	0.000	0.000	0.000	0.000
		0.051	0.000	0.181	0.000
		0.312	0.000	0.651	0.000
		0.392	0.018	0.694	0.052
		0.435	0.033	0.704	0.087
		0.482	0.074	0.679	0.169
		0.504	0.134	0.623	0.268
		0.505	0.208	0.554	0.370
		0.479	0.295	0.473	0.473
		0.431	0.399	0.385	0.578
		0.369	0.520	0.298	0.680
		0.269	0.663	0.198	0.790
		0.142	0.828	0.095	0.900
		0.077	0.913	0.049	0.949
		0.000	0.999	0.000	0.9998

Compositions of coexisting phases

		x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
t/°C	T/K (compiler)	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25.0	298.2	0.000	0.999	0.000	0.000	0.000	0.9998	0.000	0.000
		0.133	0.836	0.010	0.000	0.089	0.906	0.040	0.000
		0.320	0.591	0.020	0.000	0.246	0.737	0.077	0.000
		0.495	0.253	0.035	0.000	0.512	0.424	0.130	0.000
		0.312	0.000	0.051	0.000	0.651	0.000	0.181	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The points on the binodal curve were determined by the formation of a cloudy mixture on shaking after the addition of a known mass of one component to a mixture of known masses of the other two components. Precision weighing syringes were used as described in Ref. 1. Tie line compositions were determined by the refractive index method reported in Ref. 2 and a complementary method using the Karl Fischer titrations as reported in Ref. 3.

Source and Purity of Materials:

(1) Merck, AR grade; distilled, dried by the addition of anhydrous potassium carbonate, distilled; purity better than 99.6 mole % by glc.
(2) BDH; used as received; purity better than 99.6 mole % by glc.
(3) not specified.

Estimated Error:

estimated comp. 0.005 mole fraction on the binodal curve and 0.01 mole fraction for tie lines (estimated by the authors).

References:

[1] T. M. Letcher, S. Wootten, B. Shuttleworth, and C. Heward, J. Chem. Thermodyn. **18**, 1037 (1986).
[2] S. W. Briggs and F. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).
[3] T. M. Letcher, P. M. Siswana, P. Van der Watt, and S. Radloff, J. Chem. Thermodyn. **21**, 1053 (1989).

11. 3-Methyl-3-buten-1-ol+Water

Components:

(1) 3-Methyl-3-buten-1-ol; $C_5H_{10}O$; [763-32-6]
(2) 2-Methyl-1,3-butadiene (isoprene, isopentadiene); C_5H_8; [78-79-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

Yu. M. Blazhin. S. K. Ogorodnikov, A. I. Morozova, L. N. Volkova, L. V. Artem'eva, and N. S. Bad'ina, Zh, Prikl. Khim. (Leningrad) **47**, 1103–6 (1974) [Eng. transl. Russ. J. Appl. Chem. (Leningrad) **47**, 1128–30 (1974)].

Variables:

T/K=288

Compiled by:

A. Skrzecz

11.1. 3-Methyl-3-buten-1-ol + Water + 2-Methyl-1, 3-butadiene

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)		hydrocarbon-rich phase		water-rich phase	
15.0	288.15	0.5234	0.0000	0.0191	0.0000	0.840	0.000	0.085	0.000
		0.5077	0.1361	0.0169	0.0003	0.736	0.156	0.076	0.001
		0.4885	0.2041	0.0157	0.0003	0.684	0.226	0.071	0.001
		0.4554	0.2964	0.0141	0.0003	0.614	0.316	0.064	0.001
		0.3588	0.5265	0.0118	0.0003	0.449	0.521	0.054	0.001
		0.2802	0.6356	0.0107	0.0003	0.350	0.628	0.049	0.001
		0.2816	0.6487	0.0107	0.0003	0.348	0.634	0.049	0.001
		0.2117	0.7419	0.0095	0.0003	0.262	0.726	0.044	0.001

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Two-phase mixtures of known composition were placed into a thermostat and shaken for 30 min. After separation both phases were analyzed by glc.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

temp. ±0.1 °C.

12. 1-Pentanol+Water

Components:

(1) 1-Pentanol (pentyl alcohol, amyl alcohol, *n*-amyl alcohol); $C_5H_{12}O$; [71-41-0]
(2) Benzene: C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. A. K. Staveley, R. G. S. Johns, and B. C. Moore, J. Chem. Soc. 2516–23 (1951).

Variables:

T/K=284–341

Complied by:

A. Skrzecz

12.1. 1-Pentanol + Water + Benzene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
17.2	290.35	0.006 98	0.990 830	0.007 886	0.991 493
27.8	300.95	0.006 98	0.989 217	0.007 893	0.991 228
38.0	311.15	0.006 98	0.987 591	0.007 903	0.990 841
48.2	321.35	0.006 98	0.985 602	0.007 915	0.990 366
57.8	330.95	0.006 98	0.983 010	0.007 931	0.989 745
12.8	285.95	0.0119	0.985 174	0.013 439	0.985 886
17.9	291.05	0.0119	0.984 706	0.013 443	0.985 773
22.7	295.85	0.0119	0.984 173	0.013 449	0.985 644
31.7	304.85	0.0119	0.983 005	0.013 461	0.985 361
36.3	309.45	0.0119	0.982 172	0.013 470	0.985 159
41.9	315.05	0.0119	0.981 037	0.013 482	0.984 883
49.6	322.75	0.0119	0.979 064	0.013 502	0.984 403
56.7	329.85	0.0119	0.977 020	0.013 524	0.983 903
15.0	288.15	0.0223	0.973 897	0.025 167	0.973 956
15.4	288.55	0.0223	0.973 863	0.025 167	0.973 948
23.2	296.35	0.0223	0.972 861	0.025 187	0.973 696
30.4	303.55	0.0223	0.971 906	0.025 205	0.973 456
37.6	310.75	0.0223	0.970 902	0.025 225	0.973 204
37.9	311.05	0.0223	0.970 753	0.025 228	0.973 166
47.3	320.45	0.0223	0.968 898	0.025 264	0.972 698
58.3	331.45	0.0223	0.966 120	0.025 318	0.971 995
16.7	289.85	0.0281	0.966 134	0.031 737	0.966 933
17.4	290.55	0.0281	0.966 047	0.031 739	0.966 910
29.0	302.15	0.0281	0.964 932	0.031 766	0.966 624
37.4	310.55	0.0281	0.964 059	0.031 787	0.966 400
45.0	318.15	0.0281	0.963 049	0.031 812	0.966 140
51.8	324.95	0.0281	0.962 049	0.031 837	0.965 882
18.1	291.25	0.0486	0.943 586	0.054 831	0.943 367
31.2	304.35	0.0486	0.941 986	0.054 899	0.942 928
43.1	316.25	0.0486	0.940 190	0.054 975	0.942 433
52.0	325.15	0.0486	0.938 650	0.055 040	0.942 009
68.0	341.15	0.0486	0.936 460	0.055 134	0.941 403
11.2	284.35	0.084 25	0.904 960	0.094 835	0.902 683
28.4	301.55	0.084 25	0.902 230	0.095 034	0.901 849
43.3	316.45	0.084 25	0.899 660	0.095 223	0.901 061
57.8	330.95	0.084 25	0.896 850	0.095 429	0.900 196

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Mixtures were prepared in a closed apparatus; components were degassed by repeated freezing, evacuation and melting; a known amount of each component was introduced into a tube by condensation and the tube was sealed. The volume of each tube was about 30 mL.

Source and Purity of Materials:

(1) source not specified; dried by refluxing over freshly-ignited lime, and then with aluminum amalgam, distilled.
(2) source not specified; chemically purified, crystallized, distilled, dried over phosphoric anhydride.
(3) not specified.

Estimated Error:

composition $<0.2\%$; temp. <0.2 °C.

Components:

(1) 1-Pentanol (pentyl alcohol, *n*-amyl alcohol); $C_5H_{12}O$; [71-41-0]
(2) Hexane ($n=$hexane); C_6H_{14}; [110-54-3]
(3) Water; H_20; [7732-18-5]

Evaluated by:

A. Skrzecz, A. Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1995.09)

12.2. 1-Pentanol + Water + Hexane

Critical Evaluation:

A survey of reported compositions along, the saturation curve (sat.) and compositions of coexisting phases in equilibrium (eq.) for the system 1-pentanol–hexane–water is given in Table 83.

TABLE 83. Summary of experimental data for the system 1-pentanol–hexane–water

Author(s)	T/K	Type of data[a]	Ref.
Charykov *et al.*, 1978	293	sat. (7)	1
Gorovits *et al.*, 1986	298–338	eq. (39)	2

[a] Number of experimental points in parentheses.

Saturation curve

The ternary system 1-pentanol–hexane–water forms a miscibility gap of type 2. The system 1-pentanol–hexane is miscible. Two binary systems hexane–water and 1-pentanol–water, form miscibility gaps. Data for these binary systems were complied and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. The recommended values of mutual solubility at 293 K are: for hexane–water system $x_2''=2.5.10^{-6}$ and $x_2'=0.999\ 47$,[3] and for 1-pentanol–water system $x_1'=0.679$ and $x_1''=0.004\ 81$.[4] Solubility of water in hexane reported by Charykov *et al.*,[1] ($x_2'=0.9996$) is slightly smaller than the recommended value, Ref. 3, while the solubility of water in 1-pentanol ($x_1'=0.67$) is in qualitative agreement with Ref. 4. Similarly, the solubility of water in 1-pentanol at 298 K reported by Gorovits *et al.*,[2] ($x_1'=0.0666$), differs a little from that recommended in Ref. 4. ($x_1'=0.674$). The differences are within experimental error. Equilibrium data of Gorovits *et al.*[2] were taken into account during discussion of the binodal curve at temperature range 298.2–338.2 K and are self-consistent showing slightly increasing solubility with temperature. Solubility data of Charykov *et al.*[1] at 293.2 K show a slightly higher solubility at high hexane concentrations than data of Ref. 2, measured at even higher temperatures. However, these differences are within the likely experimental errors. One experimental saturation point reported in Ref. 1, ($x_1=0.73$, $x_2=0.016$) appears to be in error. Both data sets are treated as tentative.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 1-pentanol–hexane–water were reported by Gorovits *et al.*,[2] at three temperatures 298.2, 318.2, 338.2 K as well as at isobaric conditions at the pressure 16.13 kPa. All tie lines constructed on the basis of experimental points are consistent with one another. The assumption made in Ref. 2, that the concentration of hexane in the water-rich phase is negligible may be acceptable because of the very low hexane concentrations and accuracy of analytical method. The equilibrium data are treated as tentative. As an example of the system behavior, the experimental data at 298.2 K, Ref. 2, are presented in Fig. 45.

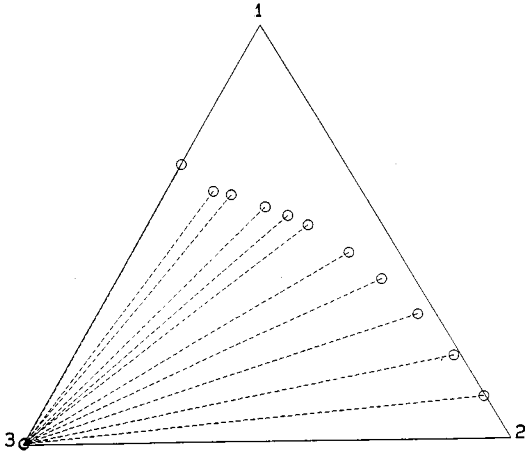

FIG. 45. Phase diagram of the system 1-pentanol (1)—hexane (2)—water (3) at 298.2 K. ○—experimental results, Ref. 2, dashed lines—experimental tie line, Ref. 2.

References:

[1] A. K. Charykov, V. I. Tikhomirov, and T. M. Potapoya, Zh. Obshch. Khim, **48**, 1916 (1978).

[2] B. I. Gorovits, N. P. Markuzin, and T. M. Lesteva, Vestn. Leningr. Univ., Ser. 4: Fiz. Khim. **4**, 100 (1986).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37, Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 and C_7 (Pergamon, New York, 1989).

[4] A . F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 1-Pentanol (pentyl alcohol, amyl alcohol, *n*-amyl alcohol); $C_5H_{12}O$; [71-41-0]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. K. Charykov, V. I. Tikhomirov, and T. M. Potapova, Zh. Obshch. Khim. **48**, 1916-21 (1978). [Eng. transl. Russ. J. Gen. Chem. **48**, 1748-50 (1978)].

Variables:

T/K=293

Compiled by:

A. Skrzecz

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
		(compiler)		(compiler)	
20	293.2	0.000	0.99954	0.000	0.99990
		0.103	0.886	0.106	0.892
		0.207	0.761	0.216	0.777
		0.389	0.522	0.424	0.556
		0.530	0.320	0.607	0.358
		0.735	0.016	0.917	0.020
		0.669	0.000	0.908	0.000

Auxiliary Information

Method/Apparatus/Procedure:

Water solubility was determined by the analytical method. Saturated mixtures were obtained by the shaking of known volumes of reagents for 2–3 h after which the concentration of water in organic phase was determined by the Karl Fischer method. The mean of three analyses was reported. The saturation concentrations were reported in the units mole/L.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) source not specified.

Estimated Error: Not reported.

Components:

(1)1-Pentanol (pentyl alcohol, amyl alcohol, *n*-amyl alcohol); $C_5H_{12}O$; [71-41-0]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

B. I. Gorovits, N. P. Markuzin, and T. M. Lesteva, Vestn. Leningr. Univ., Ser. 4: Fiz. Khim. **4**, 100-2 (1986).

Variables:

T/K=298-338

Compiled by:

A. Skrzecz

Experimental Data

Composition of coexisting phases

T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''	p/kPa
	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)		
298.2	0.102	0.8940	0.0013	0.000 02	0.1044	0.8947	0.006 33	0.000 10	18.00
	0.201	0.7838	0.0018	0.000 02	0.2071	0.7897	0.008 75	0.000 09	17.66
	0.301	0.6610	0.0022	0.000 02	0.3152	0.6767	0.010 67	0.000 09	—
	0.387	0.5448	0.0027	0.000 02	0.4145	0.5705	0.013 07	0.000 09	—
	0.451	0.447	0.0032	0.000 02	0.4962	0.4808	0.015 46	0.000 09	—
	0.518	0.331	0.0036	0.000 02	0.5937	0.3709	0.017 37	0.000 09	16.77
	0.541	0.279	0.0040	0.000 02	0.6361	0.3207	0.019 27	0.000 09	16.13
	0.562	0.223	0.0044	0.000 02	0.6821	0.2646	0.021 17	0.000 09	15.26
	0.592	0.139	0.0048	0.000 01	0.7562	0.1736	0.023 05	0.000 05	—
	0.601	0.098	0.0054	0.000 01	0.7925	0.1263	0.025 88	0.000 05	5.85
	0.666	0.000	0.0060	0.000 0	0.9070	0.0000	0.028 69	0.000 00	—
318.2	0.090	0.9050	0.0016	0.000 02	0.0922	0.9067	0.007 78	0.000 10	—
	0.197	0.7846	0.0021	0.000 02	0.2036	0.7926	0.010 19	0.000 09	—
	0.300	0.6599	0.0025	0.000 02	0.3147	0.6767	0.012 11	0.000 09	—
	0.386	0.5422	0.0031	0.000 02	0.4147	0.5695	0.014 99	0.000 09	—
	0.444	0.442	0.0036	0.000 02	0.4937	0.4804	0.017 37	0.000 09	—
	0.512	0.329	0.0041	0.000 02	0.5911	0.3713	0.019 74	0.000 09	—
	0.537	0.277	0.0044	0.000 02	0.6349	0.3202	0.021 17	0.000 09	38.00
	0.548	0.221	0.0052	0.000 02	0.6755	0.2663	0.024 94	0.000 09	35.99
	0.584	0.138	0.0055	0.000 01	0.7528	0.1739	0.026 35	0.000 05	34.00
	0.593	0.089	0.0059	0.000 01	0.7960	0.1168	0.028 22	0.000 05	—
	0.661	0.000	0.0066	0.00 00	0.9051	0.0000	0.031 49	0.000 00	—
338.2	0.0906	0.9030	0.0019	0.000 02	0.0930	0.9057	0.009 23	0.000 09	—
	0.199	0.7810	0.0029	0.000 02	0.2059	0.7899	0.014 03	0.000 09	—
	0.296	0.6578	0.0029	0.000 02	0.3121	0.6780	0.014 03	0.000 09	—
	0.386	0.5390	0.0034	0.000 02	0.4158	0.5677	0.016 42	0.000 09	—
	0.440	0.440	0.0040	0.000 02	0.4918	0.4808	0.019 27	0.000 09	—
	0.512	0.325	0.0044	0.000 02	0.5933	0.3681	0.021 17	0.000 09	—
	0.534	0.274	0.0048	0.000 02	0.6349	0.3185	0.023 05	0.000 09	—
	0.539	0.220	0.0056	0.000 02	0.6710	0.2677	0.026 81	0.000 09	—
	0.574	0.136	0.0059	0.000 01	0.7491	0.1735	0.028 22	0.000 05	—
	0.585	0.096	0.0063	0.000 01	0.7862	0.1261	0.030 09	0.000 05	—
	0.659	0.000	0.0069	0.0000	0.9044	0.0000	0.032 88	0.000 00	—

Compositions of coexisting phases at constant pressure $p=16.13$ kPa

T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''	p/kPa
	organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)		
331.3	0.660	0.000	0.0064	0.00000	0.905	0.000	0.03055	0.00000	16.13
303.3	0.581	0.139	0.0060	0.00001	0.751	0.175	0.02869	0.00005	16.13
299.6	0.559	0.221	0.0048	0.00001	0.682	0.263	0.02305	0.00005	16.13
298.2	0.541	0.279	0.0040	0.00002	0.636	0.321	0.01927	0.00009	16.13
297.2	0.511	0.335	0.0040	0.00002	0.587	0.376	0.01927	0.00009	16.13
296.4	0.448	0.447	0.0036	0.00002	0.494	0.482	0.01737	0.00009	16.13

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. After separation both phases were analyzed. Water in the organic-rich phase was analyzed by the Karl Fischer method. The samples were analyzed by glc with propanol as the internal standard. A known amount of decane (about 10% by weight) was added to the water-rich phase and then after separation, samples of upper phase were analyzed by glc (the assumption was made that there was no hexane in lower phase). Vapor pressures over the two-phase mixtures were measured by static method described in Ref. 1.

Source and Purity of Materials:

(1) source not specified; pure for analysis grade; twice distilled on a column of 20 theoretical plates, stored over zeolite; b.p.=411.2 K, $d(20\ °C,4\ °C)=0.8145$, $n(20\ °C,D)=1.4102$; the properties (b.p., *d,n*) were in agreement with literature data.
(2) source not specified; pure for analysis grade; twice distilled on the column of 20 theoretical plates, stored over zeolite; b.p. =341.9 K, $d(20\ °C,4\ °C)=0.6594$, $n(20\ °C,D)=1.3750$; the properties (b.p., *d,n*) were in agreement with literature data.
(3) distilled water.

Estimated Error:

temp. ±0.1 K; relative errors of analysis: hexane and 1-pentanol in the water-rich phase, 20%–25% and 5%–7% respectively; water in the organic-rich phase, 3%.

References:

[1] I. A. Zvereva, I. M. Balashova, and N. A. Smirnova, Vestn. Leningr. Univ., Ser. 4: Fiz. Khim. **22**, 107 (1977).

Components:
(1) 1-Pentanol (pentyl alcohol, amyl alcohol, *n*-amyl alcohol); $C_5H_{12}O$; [71-41-0]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:
T/K=298

Compiled by:
A. Skrzecz

12.3. 1-Pentanol + Water + Heptane

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.699	0.000	0.919	0.000
		0.703	0.057	0.861	0.079
		0.694	0.130	0.791	0.168
		0.640	0.228	0.691	0.280
		0.581	0.324	0.600	0.380
		0.495	0.450	0.486	0.503
		0.318	0.656	0.297	0.698
		0.110	0.884	0.099	0.900
		0.004	0.000	0.019	0.000

Compositions of coexisting phases

		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
t/°C (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
25	298.2	0.640	0.228	0.004	0.000	0.691	0.280	0.019	0.000
		0.370	0.595	0.003	0.000	0.351	0.642	0.015	0.000
		0.111	0.884	0.002	0.000	0.099	0.900	0.010	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of other two components in 100 cm^3 long-neck flask until one drop (weighing less than 0.01 g) results cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at temperature of 298.3 K to ensure that separation did not take place. The tie lines were determined from mixtures of well known composition in the immiscible region. The flasks were well shaken and left for separation. The refractive indexes of the samples of the both phases were measured and related to compositions the coexisting curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) Analytical Carlo Erba, 99 mole %; dried with anhydrous potassium carbonate, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through column containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).

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13. 2-Pentanol+Water

Components:
(1) 2-Pentanol (dl-2-pentanol, (RS)-2-pentanol); $C_5H_{12}O$; [6032-29-7]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:
T/K=298

Compiled by:
A. Skrzecz

13.1. 2-Pentanol + Water + Heptane

Experimental Data

Compositions along the saturation curve

t/SDC (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.651	0.000	0.901	0.000
		0.598	0.175	0.709	0.236
		0.500	0.358	0.534	0.435
		0.362	0.595	0.346	0.646
		0.115	0.853	0.105	0.889
		0.009	0.000	0.043	0.000

Compositions of coexisting phase

		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
t/°C (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
25	298.2	0.609	0.159	0.005	0.000	0.727	0.216	0.024	0.000
		0.390	0.530	0.004	0.000	0.387	0.597	0.019	0.000
		0.110	0.880	0.002	0.000	0.099	0.899	0.010	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) source not specified.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities in the worst case (authors).

References:

[1] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).

14. 1-Hexanol+Water

Components:

(1) 1-Hexanol (hexyl alcohol); $C_6H_{14}O$; [111-27-3]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

T. M. Letcher, S. Wootton, B. Shuttleworth, and C. Heyward, J. Chem. Thermodyn. **18**, 1037–42 (1986).

Variables:

T/K=298

Compiled By:

A. Skrzecz

14.1. 1-Hexanol + Water + Heptane

Experimental Data

Compositions along the saturation curve

t/°C (compiler)	T/K	x_1	x_2	w_1 (compiler)	w_2 (compiler)
25	298.2	0.708	0.000	0.932	0.000
		0.701	0.062	0.872	0.076
		0.625	0.227	0.715	0.255
		0.518	0.404	0.558	0.427
		0.180	0.812	0.184	0.814
		0.001	0.000	0.006	0.000

Compositions of coexisting phase

t/°C (compiler)	T/K	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		organic-rich phase		water-rich phase		organic-rich phase (compiler)		water-rich phase (compiler)	
25	298.2	0.687	0.105	0.001	0.000	0.831	0.125	0.006	0.000
		0.476	0.456	0.001	0.000	0.509	0.478	0.006	0.000
		0.097	0.897	0.001	0.000	0.099	0.099	0.006	0.000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method, adapted from Ref. 1, was used to determine the coexistence curve. The third component was added from a weighed gas-tight syringe to a weighed mixture of the other two components in 100 mL long-neck flask until one drop (weighing less than 0.01 g) resulted in cloudiness. The flask was immersed in a well controlled water bath and shaken continuously. Refractive indexes of these mixtures were measured at 298.3 K to ensure that separation did not take place. Tie lines were determined from mixtures of known composition in the immiscible region. The flasks were shaken well and the phases allowed to separate. Refractive indexes of samples of both phases were measured and related to compositions on the coexistence curve. Each tie line was checked to ensure that it passed through the composition of the overall mixture.

Source and Purity of Materials:

(1) Fluka, puriss. quality; dried with anhydrous potassium carbonate, filtrated, distilled.
(2) Analytical Carbo Erba, purity 99.5 mole %; purified by passing through columns containing silica gel and basic alumina.
(3) de-ionized.

Estimated Error:

composition ±0.005 mole fraction for measured points, ±0.01 mole fraction for tie-lines extremities is the worst case (authors).

References:

[1] S. W. Briggs and E. W. Comings, Ind. Eng. Chem. **35**, 411 (1943).

15. Benzyl alcohol+Water

Components:

(1) Benzyl alcohol (benzenemethanol); C_7H_8O; [100-51-6]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2; [7732-18-5]

Original Measurements:

G. G. Ivanova, T. N. Telichko, G. Ya. Kolyuchkina, V. S. Timofeev, and L. A. Serafimov, Tr. Inst.-Mosk. Inst. Tonkoi Khim. Tekhnol. im. M. V. Lomonosova **3(1)**, 88–94 (1973).

Variables:

T/K=373–298

Compiled by:

A. Skrzecz

15.1. Benzyl alcohol + Water + Hexane

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
20	293.2	0.008	0.990	0.002	<0.001	0.010	0.989	0.012	0.000
		0.013	0.984	0.003	<0.001	0.016	0.983	0.018	0.000
		0.020	0.975	0.005	<0.001	0.025	0.974	0.029	0.000[a]
62.2	335.4	0.019	0.978	0.002	<0.001	0.024	0.976	0.012	0.000[b]
62.8	336.0	0.034	0.960	0.003	<0.001	0.042	0.956	0.018	0.000[b]
63.1	336.3	0.050	0.940	0.004	<0.001	0.062	0.935	0.023	0.000[b]
63.4	336.6	0.063	0.921	0.005	<0.001	0.079	0.918	0.029	0.000[a]

Compositions of coexisting phases

t/°C	T/K (compiler)	x'''_1	x'''_2	x''_1	x''_2	w'''_1	w'''_2	w''_1	w''_2
		alcohol-rich phase		water-rich phase		alcohol-rich phase (compiler)		water-rich phase (compiler)	
20	293.2	0.879	0.000	0.005	0.000	0.978	0.000	0.029	0.000
		0.830	0.009	0.005	<0.001	0.961	0.008	0.029	0.000
		0.768	0.020	0.005	<0.001	0.937	0.019	0.029	0.000
		0.707	0.028	0.005	<0.001	0.914	0.029	0.029	0.000
		0.668	0.032	0.005	<0.001	0.898	0.034	0.029	0.000[a]
99.9	373.1	0.420	0.000	0.005	<0.001	0.813	0.000	0.029	0.000[c]
92	365	0.458	0.021	0.005	<0.001	0.816	0.030	0.029	0.000[c]
82	355	0.491	0.044	0.005	<0.001	0.813	0.058	0.029	0.000[c]
72	345	0.513	0.067	0.005	<0.001	0.806	0.084	0.029	0.000[c]
63.4	336.6	0.529	0.089	0.005	<0.001	0.797	0.107	0.029	0.000[a]

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x'''_1	x'''_2	w'_1	w'_2	w'''_1	w'''_2
		hydrocarbon-rich phase		alcohol-rich phase		hydrocarbon-rich phase (compiler)		alcohol-rich phase (compiler)	
20	293.2	0.052	0.948	0.817	0.183	0.064	0.936	0.849	0.151
		0.040	0.958	0.798	0.099	0.050	0.950	0.892	0.088
		0.034	0.963	0.780	0.056	0.042	0.957	0.915	0.052
		0.028	0.968	0.731	0.039	0.035	0.964	0.913	0.039
		0.025	0.970	0.700	0.037	0.031	0.968	0.905	0.038
		0.020	0.975	0.668	0.032	0.025	0.974	0.898	0.034[a]
67.0	340.2	0.090	0.895	0.631	0.220	0.112	0.885	0.759	0.211[b]
66.0	339.2	0.084	0.901	0.623	0.157	0.104	0.892	0.794	0.159[b]
65.3	338.5	0.082	0.903	0.599	0.138	0.102	0.895	0.796	0.146[b]
64.5	337.7	0.070	0.915	0.569	0.119	0.087	0.910	0.795	0.132[b]
64.0	337.2	0.068	0.916	0.550	0.104	0.085	0.912	0.796	0.120[b]
63.4	336.6	0.063	0.921	0.529	0.089	0.079	0.918	0.797	0.107[a]

[a] Three liquid phases in equilibrium.

[b,c] Boiling temperature estimated by the compiler; (b) ±0.5 K; (c) ±5 K.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Composition of samples was determined by glc analysis with 2-propanol as an inert standard. (Column: 1.8 m×5 mm internal diameter, 10% squalane on polichromom, temp. 130 °C, H_2−9 L/h). Solubility at 293 K was determined by Alekseev's method; at boiling point in the apparatus reported in Ref. 1. The three liquid phases in equilibrium were observed in the system.

Source and Purity of Materials:

(1) source not specified, ''chromatographic purity;'' used as received; $n(20\ °C,D)=1.5401$, b.p.=205.20 °C.
(2) source not specified, ''chromatographic purity;'' used as received; $n(20\ °C,D)=1.3747$, b.p.=68.70 °C.
(3) doubly distilled.

Estimated Error:

concentration ±0.5% of glc analysis.

References:

[1] G. Ya. Kolyuchkina, V. S. Timofeev, and L. A. Serafimov, Tr. Inst.-Mosk. Inst. Tonkoi Khim. Tekhnol. im. M. V. Lomonosova **1(3)**, 65 (1971).

Components:

(1) Benzyl alcohol (benzenemethanol); C_7H_8O; [100-51-6]
(2) Toluene (methylbenzene); C_7H_8; [108-88-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

M. P. Susarev and A. I. Gorbunov, Zh. Prikl. Khim. (Leningrad) **36**, 459–61 (1963). [Eng. transl. Russ. J. Appl. Chem. (Leningrad) **56,** 197–9 (1963)].

Variables:

T/K=293–373

Compiled by:

A. Skrzecz

15.2. Benzyl alcohol + Water + Toluene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	m_a	m_b	x_1	x_2	w_1	w_2
				(compiler)		(compiler)	
20	293.2	30.0	0.8a)	0.2564	0.7022	0.2976	0.6944
		40.0	1.6a)	0.3328	0.5859	0.3936	0.5904
		50.0	2.3 a	0.4071	0.4778	0.4885	0.4885
		60.0	2.8a)	0.4830	0.3779	0.5832	0.3888
		70.0	4.0a)	0.5376	0.2704	0.6720	0.2880
		80.0	5.5a)	0.5780	0.1696	0.7560	0.1890
		90.0	7.2a)	0.6069	0.0791	0.8352	0.0928
		100.0	9.2a)	0.6218	0.0000	0.9080	0.0000
		50.0	99.8b)	0.0002	0.0002	0.0010	0.0010
		60.0	99.7b)	0.0003	0.0002	0.0018	0.0012
		70.0	99.6b)	0.0005	0.0002	0.0028	0.0012
		80.0	98.8b)	0.0016	0.0005	0.0096	0.0024
		90.0	98.1b)	0.0029	0.0004	0.0171	0.0019
		100.0	95.8b)	0.0073	0.0000	0.0420	0.0000

Compositions of coexisting phases

t/°C	T/K (compiler)	x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
		organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
87.0	360.2	0.1813	0.8082	0.0071	0.0008	0.208	0.790	0.041	0.004
87.7	360.9	0.2544	0.6846	0.0073	0.0008	0.300	0.688	0.042	0.004
88.0	361.2	0.3223	0.5553	0.0082	0.0008	0.395	0.580	0.047	0.004
88.0	361.2	0.3770	0.4279	0.0093	0.0008	0.487	0.471	0.053	0.004
88.6	361.8	0.4201	0.3158	0.0100	0.0008	0.573	0.367	0.057	0.004
89.7	362.9	0.4652	0.2212	0.0119	0.0006	0.659	0.267	0.067	0.003
91.9	365.1	0.4629	0.1347	0.0137	0.0006	0.718	0.178	0.077	0.003
95.9	369.1	0.4493	0.0543	0.0145	0.0004	0.777	0.080	0.081	0.002
97.6	370.8	0.4096	0.0221	0.0149	0.0002	0.783	0.036	0.083	0.001
100.0	373.2	0.3810	0.0000	0.0150	0.0000	0.787	0.000	0.084	0.000

m_a—alcohol concentration (mass %) in binary benzyl alcohol–toluene mixture.

m_b—water concentration (mass %): (a) in organic-rich phase; (b) in water-rich phase.

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used to measure solubility curve at 20 °C. Binary benzyl alcohol–toluene mixtures were titrated with water and water was titrated with binary benzyl alcohol–toluene mixtures. The analytical method was used to determine liquid–liquid–vapor equilibrium (LLVE) data at boiling temperature at 101.32 kPa. Samples of hot liquid organic rich phase taken from the apparatus were cooled to 20 °C and titrated with a binary benzyl alcohol–toluene mixture (the mixture composition was the same as used to prepare the primary sample for LLVE measurements) until homogenization was obtained. The assumption was made that the ratio of benzyl alcohol to toluene in hot liquid phase was the same as at the beginning of experiment in binary mixture. The fraction of water rich phase was always small. The concentration was calculated from mass balance.

Source and Purity of Materials:

(1) source not specified; purified; b.p.=205.5 °C, $n(20\ °\mathrm{C,D})=1.5406$, $d(20\ °\mathrm{C},4\ °\mathrm{C})=1.0459$.
(2) source not specified; purified; b.p.=110.6 °C, $n(20\ °\mathrm{C,D})=1.4968$, $d(20\ °\mathrm{C},4\ °\mathrm{C})=0.8670$.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) Benzyl alcohol (benzenemethanol); C_7H_8O; [100-51-6]
(2) Heptane (*n*- heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

G. G. Ivanova, T. N. Telichko, G. Ya. Kolyuchkina, V. S. Timofeev, and L. A. Serafimov, Tr. Inst.-Mosk. Inst. Tonkoi Khim. Tekhnol. im. M. V. Lomonosova **3(2)**, 99–105 (1973).

Variables:

$T/\mathrm{K}=293-373$

Compiled by:

A. Skrzecz

15.3. Benzyl alcohol + Water + Heptane

Experimental Data

Compositions of coexisting phases

$t/°\mathrm{C}$	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		hydrocarbon-rich phase		water-rich phase		hydrocarbon-rich phase (compiler)		water-rich phase (compiler)	
20	293.2	0.006	0.992	0.002	0.000	0.006	0.993	0.012	0.000
		0.012	0.985	0.003	0.000	0.013	0.986	0.018	0.000
		0.017	0.979	0.005	0.000	0.018	0.981	0.029	0.000^a
79.4	352.6	0.031	0.960	0.002	0.000	0.034	0.965	0.012	0.000^b
	352.6	0.052	0.929	0.003	0.000	0.057	0.940	0.018	0.000^b
	352.6	0.068	0.904	0.004	0.000	0.075	0.920	0.024	0.000^b
79.7	352.9	0.081	0.879	0.005	0.000	0.090	0.903	0.029	0.000^a

Compositions of coexisting phases

$t/°\mathrm{C}$	T/K (compiler)	x_1'''	x_2'''	x_1''	x_2''	w_1'''	w_2'''	w_1''	w_2''
		alcohol-rich phase		water-rich phase		alcohol-rich phase (compiler)		water-rich phase (compiler)	
20	293.2	0.879	0.000	0.005	0.000	0.978	0.000	0.029	0.000
		0.818	0.010	0.005	0.000	0.956	0.011	0.029	0.000
		0.777	0.014	0.005	0.000	0.942	0.016	0.029	0.000
		0.730	0.020	0.005	0.000	0.924	0.023	0.029	0.000
		0.678	0.028	0.005	0.000	0.900	0.034	0.029	0.000^a
100	373	0.420	0.000	0.005	0.000	0.813	0.000	0.029	0.000^c
92	365	0.450	0.010	0.005	0.000	0.819	0.017	0.029	0.000^c
89	362	0.462	0.029	0.005	0.000	0.805	0.047	0.029	0.000^c
83	356	0.480	0.050	0.005	0.000	0.794	0.077	0.029	0.000^c
79.7	352.9	0.489	0.066	0.005	0.000	0.783	0.098	0.029	0.000^a

Compositions of coexisting phases

		x'_1	x'_2	x'''_1	x'''_2	w'_1	w'_2	w'''_1	w'''_2
$t/°C$	T/K (compiler)	hydrocarbon-rich phase		alcohol-rich phase		hydrocarbon-rich phase (compiler)		alcohol-rich phase (compiler)	
20	293.2	0.049	0.951	0.847	0.153	0.053	0.947	0.857	0.143
		0.047	0.952	0.827	0.108	0.051	0.949	0.882	0.107
		0.035	0.963	0.800	0.070	0.038	0.962	0.902	0.073
		0.024	0.973	0.751	0.029	0.026	0.974	0.922	0.033
		0.017	0.979	0.678	0.028	0.018	0.981	0.900	0.034[a]
81.0	354.2	0.198	0.724	0.555	0.226	0.225	0.761	0.693	0.261[b]
80.9	354.1	0.170	0.760	0.560	0.199	0.192	0.795	0.714	0.235[b]
80.6	353.8	0.140	0.800	0.553	0.160	0.157	0.832	0.738	0.198[b]
80.2	353.4	0.113	0.837	0.540	0.133	0.126	0.865	0.752	0.172[b]
79.9	353.1	0.097	0.860	0.516	0.094	0.108	0.884	0.772	0.130[b]
79.7	352.9	0.081	0.879	0.489	0.066	0.090	0.903	0.783	0.098[a]

[a] Three liquid phases in equilibrium.

[b,c] Boiling temperature estimated by the compiler; (b) ±0.3 K; (c) ±5 K.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used Composition of samples was determined by glc analysis with 2-propanol as an inert standard. (Column: 1.8 m×5 mm internal diameter, 10% squalane on polichromom, temp. 130 °C, H_2−9 L/h). Solubility at 293 K was determined by Alekseev's method; at boiling point—in the apparatus reported in Ref. 2. The description of the method was taken from Ref. 1. Three liquid phases in equilibrium were observed in the system.

Source and Purity of Materials:

(1) source not specified, ''chromatographic purity''; used as received; $n(20\ °C,D)=1.5401$, b.p.=205.20 °C; the same as in Ref. 1.
(2) source not specified; used as received; $n(20\ °C,D)=1.3877$, b.p.=98.4 °C.
(3) doubly distilled; the same as in Ref. 1.

Estimated Error:

concentration ±0.5 % of glc analysis, Ref. 1.

References:

[1] G. G. Ivanova, T. N. Telichko, G. Ya. Kolyuchkina, V. S. Timofeev, and L. A. Serafimov, Tr. Inst.-Mosk. Inst. Tonkoi Khim Tekhnol. im. M. V. Lomonosova **3(1)**, 88 (1973).
[2] G. Ya. Kolyuchkina, V. S. Timofeev, and L. A. Serafimov, Tr. Inst.-Mosk. Inst. Tonkoi Khim. Tekhnol. im. M. V. Lomonosova **1(3)**, 65 (1971).

Components:

(1) Benzyl alcohol (benzenemethanol); C_7H_8O; [100-51-6]
(2) 1,2,3,4-Tetrahydronaphthalene (tetralin); $C_{10}H_{12}$; [119-64-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

S. Goto, M. Matsubara, and K. Washino, Kagaku Kogaku **38**, 869–73 (1974).

Variables:

$T/K=363$

Compiled by:

A. Skrzecz

15.4. Benzyl alcohol + Water + 1,2,3,4-Tetrahydronaphthalene

Experimental Data

Compositions along the saturation curve

		x_1	x_2		
$t/°C$	T/K (compiler)	(compiler)		w_1	w_2
90	363.2	0.2367	0.7227	0.2100	0.7840
		0.4347	0.4958	0.4130	0.5760
		0.5076	0.3741	0.5155	0.4645
		0.5574	0.2830	0.5994	0.3720
		0.6235	0.2034	0.6920	0.2760
		0.5909	0.1126	0.7596	0.1769
		0.5850	0.0495	0.8281	0.0857
		0.5400	0.0000	0.8757	0.0000

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
$t/°C$	T/K (compiler)	organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
90	363.2	0.0394	0.9091	0.0017	0.0003	0.0340	0.9586	0.0100	0.0019
		0.0910	0.8560	0.0028	0.0002	0.0794	0.9129	0.0168	0.0016
		0.1989	0.7505	0.0044	0.0003	0.1768	0.8157	0.0260	0.0020
		0.3930	0.5102	0.0075	0.0011	0.3805	0.6039	0.0430	0.0075
		0.5387	0.2949	0.0098	0.0003	0.5811	0.3890	0.0560	0.0020
		0.5270	0.1839	0.0107	0.0003	0.6588	0.2810	0.0607	0.0019
		0.5389	0.0247	0.0122	0.0000	0.8397	0.0470	0.0692	0.0002

Auxiliary Information

Method/Apparatus/Procedure:

The cloud point method was used to find compositions along the saturation curve. The analytical method was used to describe phases in equilibrium. The ternary samples of about 50 mL were thermostated for 1 h, then the phases were separated and the compositions were determined by glc analysis.

Source and Purity of Materials:

(1) source not specified, ''high purity'' commercial samples; used as received; purity > 99 mass % by glc.
(2) source not specified; ''high purity'' commercial samples; used as received; purity > 99 mass % by glc.
(3) distilled.

Estimated Error:

Not reported.

16. α-Methyl-benzenemethanol+Water

Components:	Original Measurements:
(1) alpha-Methyl-benzenemethanol; $C_8H_{10}O$; [98-85-1] (2) Ethylbenzene (phenylethane); C_8H_{10}; [100-41-4] (3) Water; H_2O; [7732-18-5]	A. F. Frolov, M. A. Loginova, E. A. Frolova, I. I. Skorokhodova, and Z. V. Krupina, Uch. Zap. Yaroslav. Tekhnol. Inst. **28**, 98–103 (1971).
Variables: T/K=298	**Compiled by:** A. Skrzecz

16.1. α-Methyl-benzenemethanol + Water + Ethylbenzene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
25	298.2	0.1878	0.7678	0.2180	0.7744
		0.7005	0.2124	0.7801	0.2056
		0.7841	0.1097	0.8760	0.1065
		0.7984	0.1077	0.8814	0.1033
		0.7948	0.0855	0.8963	0.0838
		0.7971	0.0752	0.9045	0.0741
		0.8648	0.0190	0.9625	0.0184
		0.8538	0.0053	0.9711	0.0052
		0.9347	0.0000	0.9898	0.0000
		0.0011	0.0000	0.0072	0.0000

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Samples were titrated until turbidity was observed.

Source and Purity of Materials:

(1) source not specified; b.p.=205.0 °C, $d(20\ °C,4\ °C)=1.0153$; $n(20\ °C,D)=1.5214$.
(2) source not specified; b.p.=138.5 °C, $d(20\ °C,4\ °C)=0.867$; $n(20\ °C,D)=1.4958$.
(3) distilled.

Estimated Error:

Note reported.

17. 2-Ethyl-1-hexanol+Water

Components:	Original Measurements:
(1)2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7] (2) Heaxne (n-hexane); C_6H_{14}; [110-54-3] (3) Water; H_2O; [7732-18-5]	A. M. Kiryukhin, T. M. Lesteva, and N. P. Markuzin, Prom-st Sint. Kauch. **12**, 12-4 (1981).
Variables: T/K=293–313	**Compiled by:** A. Skrzecz

17.1. 2-Ethyl-1-hexanol + Water + Hexane

Experimental Data

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t/°C (compiler)	T/K	organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25	293.2	0.0000	0.9995	0.000 000 0	0.000 007 1	0.0000	0.9999	0.000 00	0.000 034
		0.165	0.825	0.000 037 9	0.000 006 9	0.209	0.789	0.000 24	0.000 013
		0.302	0.667	0.000 063 1	0.000 005 9	0.373	0.621	0.000 40	0.000 028
		0.311	0.658	0.000 078 9	0.000 005 6	0.383	0.611	0.000 50	0.000 027
		0.373	0.580	0.000 088 4	0.000 005 4	0.456	0.535	0.000 56	0.000 026
		0.492	0.444	0.000 096 3	0.000 004 2	0.588	0.400	0.000 61	0.000 020
		0.541	0.384	0.000 099 4	0.000 003 8	0.642	0.344	0.000 63	0.000 018
		0.645	0.247	0.000 105 7	0.000 001 1	0.760	0.220	0.000 67	0.000 015
		0.710	0.165	0.000 110 5	0.000 002 5	0.831	0.146	0.000 70	0.000 012
		0.789	0.078	0.000 112 0	0.000 002 1	0.908	0.068	0.000 71	0.000 010
		0.836	0.000	0.000 123 1	0.000 000 0	0.970	0.000	0.000 78	0.000 000
40	313.2	0.0000	0.9995	0.000 000 0	0.000 010 7	0.0000	0.9999	0.000 00	0.000 051
		0.177	0.808	0.000 045 7	0.000 010 0	0.224	0.773	0.000 29	0.000 048
		0.311	0.673	0.000 050 5	0.000 009 4	0.379	0.618	0.000 32	0.000 045
		0.382	0.582	0.000 075 7	0.000 008 4	0.462	0.531	0.000 48	0.000 040
		0.447	0.495	0.000 086 8	0.000 006 7	0.539	0.450	0.000 55	0.000 012
		0.504	0.427	0.000 099 4	0.000 006 3	0.602	0.385	0.000 63	0.000 030
		0.590	0.319	0.000 115 2	0.000 004 2	0.698	0.285	0.000 73	0.000 020
		0.668	0.228	0.000 121 5	0.000 003 8	0.780	0.201	0.000 77	0.000 018
		0.713	0.167	0.000 129 4	0.000 002 1	0.831	0.147	0.000 82	0.000 010
		0.8480	0.0000	0.000 115 7	0.000 000 0	0.9725	0.000	0.000 86	0.000 000

Auxiliary Information

Method/Apparatus/Procedure:

After separation both phases were analyzed. Concentrations of organic components were determined by glc; water was determined by the Karl Fischer method. To determine hydrocarbon in the water-rich phase, samples were extracted by nonane.

Source and Purity of Materials:

(1) source not specified; distilled, dried over zeolite; purity > 99.9 % mass.
(2) source not specified; distilled; purity > 99.9 % mass.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) 2-Ethyl-1-hexanol; $C_8H_{18}O$; [104-76-7]
(2) Decahydronaphthalene (cis+trans) (decalin, bicyclo[4.4.0]decane); $C_{10}H_{18}$; [91-17-8]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

F. Ruiz, V. Gomis and R. F. Botella, Fluid Phase Equilib. **43**, 317–27 (1988).

Variables:

T/K=298

Compiled by:

A. Skrzecz

17.2. + 2-Ethyl-1-hexanol + Water + Decahydronaphthalene (cis+trans)

Experimental Data

Compositions of coexisting phases

t/°C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_3'	w_1''	w_2''
		organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase			water-rich phase	
25.0	298.2	0.864	0.000	0.000 134	0.000 00	0.976	0.000	0.0242	0.000 85	0.999[a]
		0.745	0.155	0.000 110	0.000 00	0.786	0.198	0.0167	0.000 70	0.999
		0.599	0.331	0.000 093	0.000 00	0.593	0.396	0.0110	0.000 59	0.999
		0.427	0.531	0.000 066	0.000 00	0.397	0.597	0.0061	0.000 42	1.000
		0.227	0.754	0.000 063	0.000 00	0.199	0.798	0.0026	0.000 40	1.000
		0.000	1.000	0.000 000	0.000 00	0.000	1.000	0.0000	0.000 00	1.000[b]

[a] Result of phase equilibria measurement of binary system 2-ethyl-1-hexanol–water.
[b] Result of phase equilibria measurement of binary system decahydronaphthalene–water.

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. Mixtures of known overall composition, by weight, were stirred intensely and allowed to settle for 2 h at constant temperature bath. Samples of each phase were taken and analyzed by glc method with 1-propanol as internal standard. (1-Propanol also prevented phase separation.) Analytical conditions: column 2 m×3 mm, packed with Chromosorb 101 100/120, temp. 190 °C, thermal conductivity detector for the organic phase, flame ionization detector for aqueous phase, helium flow rate—40 mL/min. Decahydronaphthalene was reported to be undetectable in the organic phase.

Source and Purity of Materials:

(1) Merck; used as received; <0.2 wt % impurities by glc.
(2) Merck; used as received; mixture of cis- and trans- isomers.
(3) not reported.

Estimated Error:

temp ±0.1 °C.

18. 1-Octanol+Water

Components:

(1) 1-Octanol (octyl alcohol, capryl alcohol); $C_8H_{18}O$; [111-87-5]
(2) Pentane (n-pentane); C_5H_{12}; [109-66-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Kiryukhin,T. M. Lesteva, and N. P. Markuzin, Prom-st Sint. Kauch. **12**, 12-4 (1981).

Variables:

T/K=293

Compiled by:

A. Skrzecz

18.1. 1-Octanol + Water + Pentane

Experimental Data

Compositions of coexisting phase

t/°C (compiler)	T/K	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		organic-rich phase (compiler)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25	293.2	0.000	0.999736	0.000 000 0	0.000 012 0	0.000	0.999 934	0.000 00	0.000 048
		0.164	0.809	0.000 011 1	0.000 011 2	0.266	0.728	0.000 08	0.000 045
		0.273	0.680	0.000 027 7	0.000 009 2	0.416	0.574	0.000 20	0.000 037
		0.425	0.528	0.000 034 6	0.000 007 2	0.587	0.404	0.000 25	0.000 029
		0.455	0.442	0.000 038 7	0.000 006 5	0.637	0.343	0.000 28	0.000 026
		0.474	0.412	0.000 038 7	0.000 006 2	0.660	0.318	0.000 28	0.000 025
		0.541	0.366	0.000 041 5	0.000 004 7	0.715	0.268	0.000 30	0.000 019
		0.563	0.262	0.000 048 4	0.000 004 2	0.769	0.198	0.000 35	0.000 017
		0.655	0.131	0.000 052 6	0.000 004 0	0.865	0.096	0.000 38	0.000 016
		0.709	0.040	0.000 056 7	0.000 004 0	0.926	0.028	0.000 41	0.000 016
		0.742	0.000	0.000 058 1	0.000 000 0	0.954	0.000	0.000 42	0.000 000

Auxiliary Information

Method/Apparatus/Procedure:

After separation both phases were analyzed. Concentrations of organic components were determined by glc; water was determined by the Karl Fischer method. To determine hydrocarbon in the water-rich phase, samples were extracted by nonane.

Source and Purity of Materials:

(1) soruce not specified; distilled, dried over zeolite; purity >99.9% mass.
(2) source not specified; distilled; purity >99.9% mass.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) 1-Octanol (octyl alcohol, capryl alcohol); $C_8H_{18}O$; [111-87-5]
(2) Benzene; C_6H_6; [71-43-2]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. A. K. Staveley, R. G. S. Johns, and B. C. Moore, J. Chem. Soc. 2516–23 (1951).

Variables:

T/K=287–335

Compiled by:

A. Skrzecz

18.2. 1-Octanol + Water + Benzene

Experimental Data

Compositions along the saturation curve

t/°C	T/K (compiler)	x_1	x_2	w_1	w_2
				(compiler)	
22.5	295.65	0.0166	0.980 665	0.027 429	0.971 946
31.0	304.15	0.0166	0.979 665	0.027 450	0.971 695
33.0	306.15	0.0166	0.979 045	0.027 463	0.971 540
49.5	322.65	0.0166	0.977 116	0.027 504	0.971 056
62.1	335.25	0.0166	0.974 844	0.027 552	0.970 484
14.3	287.45	0.0314	0.965 007	0.051 415	0.947 771
23.7	296.85	0.0314	0.964 079	0.051 451	0.947 524
28.4	301.55	0.0314	0.963 248	0.051 483	0.947 303
41.65	314.80	0.0314	0.961 400	0.051 555	0.946 809
26.0	299.15	0.0435	0.950 801	0.070 779	0.927 938
33.5	306.65	0.0435	0.949 879	0.070 828	0.927 681
35.8	308.95	0.0435	0.949 242	0.070 862	0.927 503
38.9	312.05	0.0435	0.948 548	0.700 899	0.927 308
46.7	319.85	0.0435	0.947 152	0.070 973	0.926 917
53.4	326.55	0.0435	0.945 450	0.071 064	0.926 438

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method was used. Water was introduced into a tube by condensation of a known amount of vapor; the required amount of the octanol–benzene solution was siphoned into a tube which was then sealed.

Source and Purity of Materials:

(1) soruce not specified; dried by refluxing over freshly ignited lime, and then with aluminum amalgam, distilled.
(2) source not specified; chemically purified, crystallized, distilled, dried over phosphoric anhydride.
(3) not specified.

Estimated Error:

composition <0.2%; temp. <0.2 °C.

Components:

(1) 1-Octanol (octyl alcohol, capryl alcohol); $C_8H_{18}O$; [111-87-5]
(2) Hexane (n-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Evaluated by:

A. Skrzecz, Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland (1996.04)

18.3. 1-Octanol + Water + Hexane

Critical Evaluation:

A survey of reported compositions along the saturation curve and compositions of coexisting phases in equilibrium (eq.) for the system 1-octanol–hexane–water is given in Table 84.

TABLE 84. Summary of experimental data for the system 1-octanol–hexane–water

Author(s)	T/k	Type of data[a]	Ref.
Kiryukhin *et al.*, 1981	293, 313	eq. (21)	1
Kiryukhin *et al.*, 1983	335–373	eq. (12)	2

[a] Number of experimental points in parentheses.

Saturation curve

The system 1-octanol–hexane–water forms a large miscibility gap of type 2 covering the majority of the concentration triangle. Compositions along the saturation curves were not reported independently in the references; the saturation curves can be constructed on the basis of equilibrium compositions of phases. Two binary systems, hexane–water and 1-octanol–water, form miscibility gaps. The data for these systems were compiled and critically evaluated in previously published SDS volumes, Refs. 3 and 4, respectively. The recommended values of mutual solubility of the hexane–water system[3] at 293 K are: $x_2'=0.99946$ and $x_2''=2.5\cdot 10^{-6}$. The recommended values of mutual solubility of 1-octanol–water system[4] at 298 K are: $x_1'=0.742$ and $x_1''=7.5\cdot 10^{-5}$. Experimental solubilities of binary systems presented in Ref. 1 at 293.2 K are: $x_1'=0.99970$, $x_2''=7.1\cdot 10^{-6}$ and $x_1'=0.742$, $x_1''=5.81\cdot 10^{-5}$, respectively.

Phases in equilibrium

Compositions of coexisting phases in equilibrium for the ternary system 1-octanol–hexane–water were reported in both references. The experimental procedure was reported very briefly in Ref. 1 and not at all in Ref. 2. All compositions of phases in equilibrium reported in Refs. 1 and 2 at various temperatures are consistent one with another. All presented data are treated as tentative. To present system behavior, experimental compositions of coexisting phases in equilibrium at 293.2 K [1] are presented in Fig. 46.

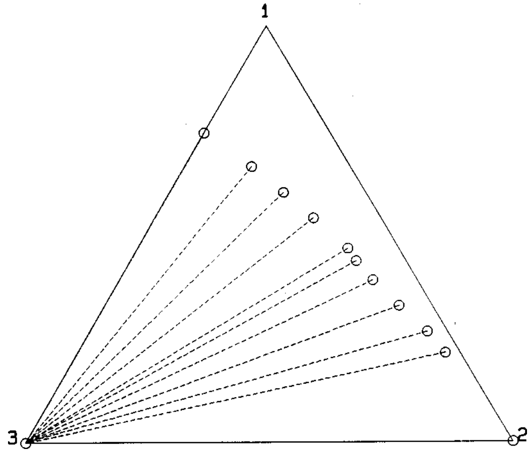

FIG. 46. Phase diagram of the system 1-octanol (1)—hexane (2)—water (3) at 293.2 K. ○—experimental data, Ref. 1, dashed lines—experimental tie lines, Ref. 1.

References:

[1] A. M. Kiryukhin, T. M. Lesteva, and N. P. Markuzin, Prom-st Sint. Kauch. **12**, 12 (1981).

[2] A. M. Kiryukhin, T. M. Lesteva, and N. P. Markuzin, Prom-st Sint. Kauch. **12**, 3 (1983).

[3] D. G. Shaw, ed., *Solubility Data Series*, Vol. 37. Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7 (Pergamon, New York, 1989).

[4] A. F. M. Barton, ed., *Solubility Data Series*, Vol. 15, Alcohols with Water (Pergamon, New York, 1984).

Components:

(1) 1-Octanol (octyl alcohol, capryl alcohol); $C_8H_{18}O$; [111-87-5]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Kiryukhin, T. M. Lesteva, and N. P. Markuzin, Prom-st Sint. Kauch. **12**, 12–4 (1981).

Variables:

$T/\mathrm{K}=293-313$

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

		x'_1	x'_2	x''_1	x''_2	w'_1	w'_2	w''_1	w''_2
t °C	T/K (compiler)	organic-rich phase (complier)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25	293.2	0.000	0.999 770	0.000 000 0	0.000 007 1	0.000	0.999 952	0.000 00	0.000 034
		0.214	0.755	0.000 009 7	0.000 006 7	0.298	0.696	0.000 07	0.000 032
		0.265	0.693	0.000 018 0	0.000 006 3	0.363	0.629	0.000 13	0.000 030
		0.327	0.604	0.000 022 1	0.000 005 6	0.444	0.543	0.000 16	0.000 027
		0.388	0.520	0.000 026 3	0.000 005 0	0.521	0.462	0.000 19	0.000 024
		0.434	0.463	0.000 029 1	0.000 004 2	0.575	0.406	0.000 21	0.000 020
		0.464	0.431	0.000 031 8	0.000 003 1	0.608	0.373	0.000 23	0.000 015
		0.536	0.325	0.000 038 7	0.000 003 6	0.696	0.279	0.000 28	0.000 017
		0.598	0.233	0.000 041 5	0.000 002 1	0.771	0.199	0.000 30	0.000 010
		0.661	0.137	0.000 048 4	0.000 001 7	0.848	0.116	0.000 35	0.000 008
		0.742	0.000	0.000 058 1	0.000 000 0	0.954	0.000	0.000 42	0.000 000
40	313.2	0.000	0.9995	0.000 000 0	0.000 010 7	0.000	0.9999	0.000 00	0.000 051
		0.272	0.676	0.000 016 6	0.000 007 7	0.374	0.616	0.000 12	0.000 037
		0.357	0.563	0.000 029 1	0.000 005 9	0.482	0.503	0.000 21	0.000 028
		0.394	0.519	0.000 030 4	0.000 005 2	0.526	0.458	0.000 22	0.000 025
		0.464	0.431	0.000 037 4	0.000 004 2	0.608	0.373	0.000 27	0.000 020
		0.469	0.400	0.000 038 7	0.000 003 8	0.624	0.352	0.000 28	0.000 018
		0.545	0.320	0.000 041 5	0.000 003 1	0.703	0.273	0.000 30	0.000 015
		0.577	0.276	0.000 044 3	0.000 002 1	0.740	0.234	0.000 32	0.000 010
		0.674	0.113	0.000 055 4	0.000 000 8	0.866	0.096	0.000 40	0.000 004
		0.733	0.000	0.000 066 4	0.000 000 0	0.952	0.000	0.000 48	0.000 000

Auxiliary Information

Method/Apparatus/Procedure:

After separation both phases were analyzed. Concentrations of organic components were determined by glc; water was determined by the Karl Fischer method. To determine hydrocarbon in the water-rich phase, samples were extracted by nonane.

Source and Purity of Materials:

(1) source not specified; distilled, dried over zeolite; purity >99.9% mass.
(2) source not specified; distilled; purity >99.9% mass.
(3) not specified.

Estimated Error:

Not reported.

Components:

(1) 1-Octanol (octyl alcohol, capryl alcohol); $C_8H_{18}O$; [111-87-5]
(2) Hexane (*n*-hexane); C_6H_{14}; [110-54-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M Kiryukhim, T. M. Lesteva, and N. P. Markuzin, Prom-st Sint. Kauch. **12**, 3–6 (1983).

Variables:

p/kPa = 101.3

Compiled by:

A. Skrzecz

Experimental Data

Compositions of coexisting phases

p/kPa	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
	organic-rich phase		water-rich phase		organic-rich phase (compliier)		water-rich phase (complier)	
101.3	0.0000	0.9996	0.000 000	0.000 013	0.0000	0.9999	0.000 000	0.000 062
	0.1080	0.8785	0.000 029	0.000 025	0.1563	0.8410	0.000 210	0.000 120
	0.1990	0.7762	0.000 037	0.000 029	0.2779	0.7173	0.000 267	0.000 139
	0.2310	0.7351	0.000 040	0.000 033	0.3199	0.6736	0.000 289	0.000 158
	0.3160	0.6325	0.000 048	0.000 031	0.4261	0.5643	0.000 347	0.000 148
	0.3690	0.5575	0.000 054	0.000 027	0.4933	0.4931	0.000 390	0.000 129
	0.4380	0.4480	0.000 060	0.000 023	0.5838	0.3952	0.000 434	0.000 110
	0.5050	0.3500	0.000 062	0.000 021	0.6674	0.3061	0.000 448	0.000 100
	0.5510	0.2790	0.000 066	0.000 023	0.7258	0.2432	0.000 477	0.000 110
	0.6160	0.1670	0.000 071	0.000 019	0.8142	0.1461	0.000 513	0.000 091
	0.6700	0.0710	0.000 082	0.000 008	0.8900	0.0624	0.000 592	0.000 038
	0.7020	0.0000	0.000 090	0.000 000	0.9445	0.0000	0.000 650	0.000 000

Auxiliary Information

Method/Apparatus/Procedure:

The vapor–liquid–liquid equilibrium measurements were reported at pressure 101.3 kPa. Values of boiling temperatures were not reported. The experimental procedure was similar as in Ref. 1. No further details were reported in the paper.

Source and Purity of Materials:

(1) source not specified.
(2) source not specified.
(3) not specified.

Estimated Error:

Not reported.

References:

[1] A. M. Kiryukhin *et al.*, Prom-st Sint. Kauch. **7**, 4 (1982).

Components:

(1) 1-Octanol (octyl alcohol, capryl alcohol); $C_8H_{18}O$; [111-87-5]
(2) Heptane (*n*-heptane); C_7H_{16}; [142-82-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

A. M. Kiryukhin, T. M. Lesteva, and N. P. Markuzin, Prom-st Sint. Kauch. **12**, 12–4 (1981).

Variables: T/K = 293–333

Compiled by: A. Skrzecz

18.4. 1-Octanol + Water + Heptane

Experimental Data

Compositions of coexisting phases

t °C	T/K (compiler)	x_1'	x_2'	x_1''	x_2''	w_1'	w_2'	w_1''	w_2''
		organic-rich phase (complier)		water-rich phase (compiler)		organic-rich phase		water-rich phase	
25	293.2	0.0000	0.9994	0.000 000 0	0.000 000 5	0.0000	0.9999	0.000 00	0.000 003
		0.135	0.848	0.000 009 7	0.000 000 4	0.171	0.826	0.000 07	0.000 002
		0.277	0.676	0.000 022 1	0.000 000 4	0.345	0.647	0.000 16	0.000 002
		0.521	0.345	0.000 042 9	0.000 000 2	0.647	0.330	0.000 31	0.000 001
		0.593	0.239	0.000 048 4	0.000 000 2	0.741	0.230	0.000 35	0.000 001
		0.685	0.103	0.000 052 6	0.000 000 0	0.863	0.100	0.000 38	0.000 000
		0.742	0.000	0.000 058 1	0.000 000 0	0.954	0.000	0.000 42	0.000 000
40	313.2	0.0000	0.9994	0.000 000 0	0.000 001 1	0.0000	0.9999	0.000 00	0.000 006
		0.206	0.771	0.000 013 8	0.000 000 9	0.257	0.739	0.000 10	0.000 005
		0.369	0.567	0.000 031 8	0.000 000 7	0.453	0.536	0.000 23	0.000 004
		0.479	0.399	0.000 034 6	0.000 000 5	0.597	0.382	0.000 25	0.000 003
		0.527	0.334	0.000 038 7	0.000 000 4	0.656	0.320	0.000 28	0.000 002
		0.628	0.219	0.000 040 1	0.000 000 2	0.768	0.206	0.000 29	0.000 001
		0.659	0.175	0.000 047 0	0.000 000 2	0.807	0.165	0.000 34	0.000 001
		0.724	0.067	0.000 055 4	0.000 000 0	0.900	0.064	0.000 40	0.000 000
		0.733	0.000	0.000 066 4	0.000 000 0	0.952	0.000	0.000 48	0.000 000
60	333.2	0.0000	0.9989	0.000 000 0	0.000 002 9	0.0000	0.9998	0.000 00	0.000 016
		0.161	0.834	0.000 016 6	0.000 002 2	0.200	0.799	0.000 12	0.000 012
		0.346	0.584	0.000 027 7	0.000 001 8	0.430	0.558	0.000 20	0.000 010
		0.389	0.518	0.000 034 6	0.000 001 4	0.486	0.498	0.000 25	0.000 008
		0.441	0.454	0.000 038 7	0.000 000 9	0.548	0.434	0.000 28	0.000 005
		0.474	0.404	0.000 041 5	0.000 000 5	0.591	0.388	0.000 30	0.000 003
		0.497	0.360	0.000 044 3	0.000 000 4	0.626	0.349	0.000 32	0.000 002
		0.586	0.241	0.000 047 0	0.000 000 2	0.737	0.233	0.000 34	0.000 001
		0.676	0.112	0.000 054 0	0.000 000 0	0.854	0.109	0.000 39	0.000 000
		0.720	0.000	0.000 070 6	0.000 000 0	0.949	0.000	0.000 51	0.000 000

Auxiliary Information

Method/Apparatus/Procedure:

After separation both phases were analyzed. Concentrations of organic components were determined by glc; water was determined by the Karl Fischer method. To determine hydrocarbon in the water-rich phase, samples were extracted by nonane.

Source and Purity of Materials:

(1) source not specified; distilled, dried over zeolite; purity >99.9% mass.
(2) source not specified; distilled; purity >99.9% mass.
(3) not specified.

Estimated Error:

Not reported.

19. 1-Nonanol+Water

Components:	**Original Measurements:**
(1) 1-Nonanol (nonyl alcohol, nonanol); $C_9H_{20}O$; [143-08-8] (2) Naphthalene; $C_{10}H_8$; [91-20-3] (3) Water; H_2O; [7732-18-5]	V. P. Sazonov, M. F. Chernysheva, and A. G. Sarkisov, Zh. Prikl. Khim. (Leningrad) **52**, 2710-3 (1979). [Eng. transl. Russ. J. Appl. Chem. (Leningrad) **52,** 2565–8 (1979)].
Variables: T/K=293–333	**Compiled by:** A. Skrzecz

19.1. 1-Nonanol + Water + Naphthalene

Experimental Data

Compositions along the saturation curve

t °C	T/K (compiler)	x_1 (compiler)	x_2 (compiler)	w_1	w_2
20.0	293.2	0.740	0.000	0.958	0.000
		0.716	0.040	0.916	0.045
		0.704	0.068	0.888	0.076
		0.691	0.086	0.869	0.096[a]
		0.883	0.117	0.895	0.105[b]
		0.740	0.097	0.874	0.102[b]
23.0	296.2	0.740	0.000	0.958	0.000
		0.714	0.037	0.918	0.042
		0.695	0.066	0.887	0.075
		0.681	0.092	0.861	0.103
		0.674	0.099	0.853	0.111[a]
		0.869	0.131	0.882	0.118[b]
		0.734	0.109	0.863	0.114[b]
40.0	313.2	0.726	0.000	0.955	0.000
		0.692	0.039	0.910	0.046
		0.683	0.063	0.886	0.073
		0.668	0.089	0.859	0.102
		0.636	0.142	0.805	0.160
		0.626	0.174	0.777	0.192[a]
		0.779	0.221	0.799	0.201[b]
		0.667	0.189	0.782	0.197[b]

[a] Liquid–liquid–solid equilibrium.
[b] Liquid–solid equilibrium.

Auxiliary Information

Method/Apparatus/Procedure:

The procedure and details of the analytical method are described in Ref. 1. Equilibrium phases were analyzed by glc with a thermal conductivity detector. Glc analyses were made after separation of phases for up to 15 days. The water-rich phase contained only trace amounts of nonanol and naphthalene, therefore the experimental results were reported only as solubility data.

Source and Purity of Materials:

(1) source not specified, pure grade; dried over CaO, vacuum distilled several times; purity of the middle fraction >99 mass %; impurities—isomers and other higher alcohols.
(2) source not specified, pure for analysis grade; twice crystallized from ethanol, dried; m.p.=80.2 °C.
(3) doubly distilled.

Estimated Error:

Not reported.

References:

[1] V. P. Sazonov and M. F. Chernysheva, Zh. Prikl. Khim. (Leningrad) **51**, 1019 (1978).

20. System Index

Note: a letter E indicates presence of a Critical Evaluation

Benzene+Water
  + 1-Butanol 1186–1188E
  + 2-Butanol 1201–1202E
  + Ethanol 1027–1042E
  + Methanol 995–1002E
  + 2-Methyl-1-propanol 1165–1166E
  + 2-Methyl-2-propanol 1174–1175E
  + 1-Octanol 1223
  + 1-Pentanol 1212–1213
  + 1-Propanol 1095–1100E
  + 2-Propanol 1130–1137E
Benzyl alcohol+Water
  + Heptane 1219–1220
  + Hexane 1217–1218
  + 1, 2, 3, 4-Tetrahydronaphthalene 1220
  + Toluene 1218–1219
Butane+Water
  + 2-Butanol 1200
  + Methanol 993
1-Butanol+Water
  + Benzene 1186–1188E
  + Cyclohexane 1189–1191E
  + Heptane 1198
  + 1-Heptene 1198
  + Hexane 1191–1194E
  + Mesitylene 1199–1200
  + Toluene 1194–1197E
  + *p*-Xylene 1199
2-Butanol+Water
  + Benzene 1201–1202E
  + Butane 1200
  + Cyclohexane 1203–1205E
  + Heptane 1209
  + 1-Heptene 1209
  + Mesitylene 1211
  + Toluene 1206–1208E
  + *p*-Xylene 1210
1-Butene+Water
  + 2-Methyl-2-propanol 1173
Cyclohexane+Water
  + 1-Butanol 1189–1191E
  + 2-Butanol 1203–1205E
  + Ethanol 1045–1052E
  + Methanol 1004–1007E
  + 2-Methyl-1-propanol 1167–1169E
  + 2-Methyl-2-propanol 1176–1178E
  + 1-Propanol 1100–1103E
  + 2-Propanol 1139–1145E
Cyclohexene+Water
  + Ethanol 1043–1044E
  + Methanol 1002–1004E
  + 2-Propanol 1138
Decahydronaphthalene (cis+trans)+Water
  + Ethanol 1093–1094
  + 2-Ethyl-1-hexanol 1222
Decane+Water
  + Ethanol 1094
  + 1-Propanol 1126–1129E
2,2-Dimethylbutane+Water
  + Ethanol 1052
Ethanol+Water
  + Benzene 1027–1042E
  + Cyclohexane 1045–1052E
  + Cyclohexene 1043–1044E
  + Decahydronaphthalene (cis+trans) 1093–1094

+ Decane 1194
+ 2, 2-Dimethylbutane 1052
+ Heptane 1067–1071E
+ 1-Heptene 1066–1067
+ Hexane 1053–1058E
+ Mesitylene 1089–1091
+ Methylcyclohexane 1066
+ Nonane 1092
+ Octane 1088–1089
+ 1-Octene 1084–1085
+ Toluene 1059–1065E
+2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene 1093
+ 2, 2, 4-Trimethylpentane 1085–1088E
+ 2, 4, 4-Trimethyl-1-pentene 1084
+ *m*-Xylene 1072–1076E
+ *o*-Xylene 1077–1079E
+ *p*-Xylene 1080–1083E
Ethylbenzene+Water
+ alpha-Methyl-benzenemethanol 1221
+ 2-Propanol 1159–1160
2-Ethyl-1-hexanol+Water
+ Decahydronaphthalene (cis+trans) 1222
+ Hexane 1221
Heptane+Water
+ Benzyl alcohol 1219–1220
+ 1-Butanol 1198
+ 2-Butanol 1209
+ Ethanol 1067–1071E
+ 1-Hexanol 1217
+ Methanol 1015–1017E
+ 2-Methyl-2-propanol 1181
+ 1-Octanol 1225
+ 1-Pentanol 1216
+ 2-Pentanol 1216
+ 1-Propanol 1114–1118E
+ 2-Propanol 1153–1156E
1-Heptene+Water
+ 1-Butanol 1198
+ 2-Butanol 1209
+ Ethanol 1066–1067
+ Methanol 1014
+ 2-Methyl-1-propanol 1171
+ 2-Methyl-2-propanol 1180
+ 1-Propanol 1113
+ 2-Propanol 1153
Hexane+Water
+ Benzyl alcohol 1217–1218
+ 1-Butanol 1191–1194E
+ Ethanol 1053–1058E
+ 2+Ethyl-1-hexanol 1221
+ Methanol 1008–1011E
+ 1-Octanol 1223–1225E
+ 1-Pentanol 1213–1215E
+ 1-Propanol 1103–1108E
+ 2-Propanol 1145–1147E
1-Hexanol+Water
+ Heptane 1217
1-Hexene+Water
+ Methanol 1008
Mesitylene+Water
+ 1-Butanol 1199–1200
+ 2-Butanol 1211
+ Ethanol 1089–1091E
+ Methanol 1025–1026
+ 2-Methyl-1-propanol 1172
+ 2-Methyl-2-propanol 1185
+ 1-Propanol 1122–1123
+ 2-Propanol 1163

Methanol+Water
  + Benzene 995–1002E
  + Butane 993
  + Cyclohexane 1004–1008E
  + Cyclohexene 1002–1004E
  + Heptane 1015–1017E
  + 1-Heptene 1014
  + Hexane 1008–1011E
  + 1-Hexene 1008
  + Mesitylene 1025–1026
  + 2-Methyl-1, 3-butadiene 994
  + 1-Methylnaphthalene 1027
  + Propane 993
  + Nonane 1026
  + Octane 1023–1025E
  + Toluene 1011–1014E
  + 2,2,4-Trimethylpentane 1021–1023E
  + *p*-Xylene 1018–1019E
  + Xylene 1020
α-Methyl-benzenemethanol+Water
  + Ethylbenzene 1221
2-Methyl-1,3-butadiene+Water
  + Methanol 994
  + 3-Methyl-3-buten-1-ol 1212
3-Methyl-3-buten-1-ol+Water
  + 2-Methyl-1,3-butadiene 1212
Methylcyclohexane+Water
  + Ethanol 1066
1-Methylnaphthalene+Water
  + Methanol 1027
2-Methyl-1-propanol + Water
  + Benzene 1165–1166E
  + Cyclohexane 1067–1169E
  + 1-Heptene 1170
  + Mesitylene 1172
  + Toluene 1170
  + *p*-Xylene 1171
2-Methyl-2-propanol + Water
  + Benzene 1174–1175E
  + 1-Butene 1173
  + Cyclohexane 1176–1178E
  + Heptane 1181
  + 1-Heptene 1180
  + Mesitylene 1185
  + Tetradecane 1186
  + Toluene 1179
  + 2,2,4-Trimethylpentane 1183–1184
  + 2,4,4-Trimethylpentene 1182–1183
  + *p*-Xylene 1181–1182
Naphthalene + Water
  + 1-Nonanol 1226
Nonane + Water
  + Ethanol 1092
  + Methanol 1026
  + 1-Propanol 1123–1125E
  + 2-Propanol 1164
1-Nonanol + Water
  + Naphthalene 1226
1,7-Octadiene + Water
  + 2-Propanol 1160
Octane + Water
  + Ethanol 1088–1089
  + Methanol 1023–1025E
  + 1-Propanol 1120–1121E
  + 2-Propanol 1162
1-Octanol + Water
  + Benzene 1223
  + Hexane 1223–1225E

  + Heptane 1225
  + Pentane 1222
1-Octene + Water
  + Ethanol 1084–1085
Pentane + Water
  + 1-Octanol 1222
1-Pentanol + Water
  + Benzene 1212–1213
  + Hexane 1213–1215E
  + Heptane 1216
2-Pentanol + Water
  + Heptane 1216
Propane + Water
  + Methanol 993
1-Propanol + Water
  + Benzene 1095–1100E
  + Cyclohexane 1100–1103E
  + Decane 1126–1129E
  + Heptane 1114–1118E
  + 1-Heptene 1113
  + Hexane 1103–1108E
  + Mesitylene 1122–1123
  + Nonane 1123–1125E
  + Octane 1120–1122E
  + Toluene 1109–1113E
  + *p*-Xylene 1119
2-Propanol + Water
  + Benzene 1130–1137E
  + Cyclohexane 1139–1145E
  + Cyclohexene 1138
  + Ethylbenzene 1159–1160
  + Heptane 1153–1156E
  + 1-Heptene 1153
  + Hexane 1145–1147E
  + Mesitylene 1163
  + Nonane 1164
  + 1,7-Octadiene 1160
  + Octane 1162
  + Toluene 1148–1152E
  + 2,2,4-Trimethylpentane 1161
  + *m*-Xylene 1156–1157
  + *o*-Xylene 1157–1158
  + *p*-Xylene 1158–1159
Tetradecane + Water
  + 2-Methyl-2-propanol 1186
1,2,3,4-Tetrahydronaphthalene + Water
  + Benzyl alcohol 1220
Toluene + Water
  + Benzyl alcohol 1218–1219
  + 1-Butanol 1194–1197E
  + 2-Butanol 1206–1208E
  + Ethanol 1059–1064E
  + Methanol 1011–1014E
  + 2-Methyl-1-propanol 1170
  + 2-Methyl-2-propanol 1179
  + 1-Propanol 1109–1113E
  + 2-Propanol 1148–1152E
2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene + Water
  + Ethanol 1093
2,2,4-Trimethylpentane + Water
  + Ethanol 1085–1088E
  + Methanol 1021–1023E
  + 2-Methyl-2-propanol 1183–1184E
  + 2-Propanol 1161
2,4,4-Trimethyl-1-pentene + Water
  + Ethanol 1084
2,4,4-Trimethylpentene + Water
  + 2-Methyl-2-propanol 1182–1183

m-Xylene + Water
  + Ethanol 1072–1076E
  + 2-Propanol 1156–1157
o-Xylene + Water
  + Ethanol 1077–1079E
  + 2-Propanol 1157–1158
p-Xylene + Water
  + 1-Butanol 1199
  + 2-Butanol 1210
  + Ethanol 1080–1083E
  + Methanol 1018–1019E
  + 2-Methyl-1-propanol 1171
  + 2-Methyl-2-propanol 1181–1182
  + 1-Propanol 1119
  + 2-Propanol 1158–1159
Xylene + Water
  + Methanol 1020

21. Registry Number Index

64-17-5 1027–1094
67-56-1 993–1027
67-63-0 1130–1164
71-23-8 1095–1129
71-36-3 1186–1200
71-41-0 1212–1216
71-43-2 995–1002, 1027, 1042, 1095–1100, 1130–1137, 1165–1166, 1174–1175, 1186–1188, 1201–1202, 1212–1213, 1223
74-98-6 993
75-65-0 1173–1186
75-83-2 1052
78-79-5 994, 1212
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