IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 3. $C_6H_8 - C_6H_{12}$ Hydrocarbons with Water and Heavy Water

Volume Editors
Andrzej Maczynski[a)]
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

David G. Shaw[b)]
University of Alaska, Fairbanks, Alaska, USA

Evaluators
Marian Goral and Barbara Wisniewska-Goclowska
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Compilers
Adam Skrzecz
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Iwona Owczarek and Krystyna Blazej
Institute of Coal Chemistry, Polish Academy of Sciences, Gliwice, Poland

Marie-Claire Haulait-Pirson
University of Leuven, Leuven, Belgium

Glenn T. Hefter
Murdoch University, Perth, Australia

Zofia Maczynska
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Andrzej Szafranski
Institute of Industrial Chemistry, Warsaw, Poland

Colin L. Young
University of Melbourne, Parkville, Australia

Received 1 February 2004; revised manuscript received 1 March 2004; accepted 15 April 2004; published online 9 June 2005

[a)]Electronic mail: macz@ichf.edu.pl
[b)]Electronic mail: DavidShaw@post.harvard.edu

The mutual solubilities and related liquid–liquid equilibria of $C_6H_8-C_6H_{12}$ hydrocarbons with water and heavy water are exhaustively and critically reviewed. Reports of experimental determination of solubility in 11 chemically distinct binary systems that appeared in the primary literature prior to end of 2002 are compiled. For seven systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of the all experimental data for a given homologous series of saturated or unsaturated aliphatic hydrocarbons was used. [DOI: 10.1063/1.1796631]

Key words: $C_6H_8-C_6H_{12}$ hydrocarbons; critical evaluation; heavy water; liquid–liquid equilibria; solubility; water.

Contents

*A critical Evaluation is prepared for this system.

List of Tables

List of Figures

1. Preface

1.1. Scope of This Volume

This paper is Part 3 of a revised and updated version of an earlier compilation and evaluation of the mutual solubilities of water and hydrocarbon compounds containing five or more carbon atoms.[1,2] This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) together with new compilations based on recent and

previously overlooked reports in the peer-reviewed scientific literature prior to 2003. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators.

This revised work also includes all new evaluations for systems where two or more independent measurements of solubility have been reported. In these evaluations reported solubility values are characterized as Recommended, Tentative, Doubtful, or Rejected, based on consistency between independently determined experimental values and reference values derived from a newly developed set of smoothing equations.[3–6] Recommended values are supported by two (or more) independent experimental values and a reference value that are all in agreement. Tentative values are supported by two (or more) independent values in agreement with each other, but not with the reference value, or one experimental value in agreement with the reference value. Doubtful values are those for which a single experimental value differs from the reference value. Experimental values that differ from reference values and other experimental values are Rejected.

Detailed introductory material including explanations of the formats of compilation and evaluation, definitions of commonly used measures of solubility, the derivation of the smoothing equations used calculate reference values, and the scope of the Solubility Data Series can be found in Part 1 (Maczynski and Shaw[6]).

1.2. References for the Preface

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

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

[3] A. Maczynski, M. Goral, B. Wisniewska-Goclowska, A. Skrzecz, and D. Shaw, Monatshefte für Chemie **134**, 633 (2003).

[4] A. Maczynski, B. Wisniewska-Goclowska, and M. Goral, Recommended Liquid-Liquid Equilibrium Data, Part 1: Binary C_5-C_{11} Alkane-Water Systems, J. Phys. Chem. Ref. Data **33**(2), 549 (2004).

[5] M. Goral, B. Wisniewska-Goclowska, and A. Maczynski, Recommended Liquid-Liquid Equilibrium Data, Part 2: Binary Unsaturated Hydrocarbon-Water Systems, J. Phys. Chem. Ref. Data **33**(2), 579 (2004).

[6] A. Maczynski and D. Shaw, Editors, IUPAC-NIST Solubility Data Series, Hydrocarbons with Water and Seawater—Revised and Updated, Part 1. C_5 Hydrocarbons with Water, J. Phys. Chem. Ref. Data **34**(1), 441 (2005).

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

2.1. Nature of the Project

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

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

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

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

Formats for the compilations and critical evaluations have been standardized for all volumes, and complete details for these formats can be found in previous *Solubility Data Series* volumes, for example, Sazonov and Shaw.[1]

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

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

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

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

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

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

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

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

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

3. C_6 Hydrocarbons with Water and Heavy Water
3.1. 1,4-Cyclohexadiene*

Components:
(1) 1,4-Cyclohexadiene; C_6H_8; [628-41-1]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of 1,4-Cyclohexadiene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by McAuliffe[1] at 298 K and Pierotti and Liabastre[2] at 278 K–318 K.

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

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

where: $\ln x_{1,\min} = -8.43$; $\Delta_{sln}C_P/R = 33.7$; $T_{\min} = 298$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference data are listed in Table 1. Since only one experimental data point is available at each temperature, no data can be Recommended. The data of McAuliffe[1] and Pierotti and Liabastre[2] are in good agreement with the reference data and are Tentative.

TABLE 1. Experimental values for solubility of 1,4-cyclohexadiene (1) in water (2)

T/K	Experimental values x_1 (T=tentative)	Reference values $x_1 \pm 30\%$
278.3	$1.91 \cdot 10^{-4}$ (T; Ref. 2)	$2.4 \cdot 10^{-4}$
288.4	$2.15 \cdot 10^{-4}$ (T; Ref. 2)	$2.2 \cdot 10^{-4}$
298.2	$1.57 \cdot 10^{-4}$ (T; Ref. 1)	$2.2 \cdot 10^{-4}$
298.3	$2.10 \cdot 10^{-4}$ (T; Ref. 2)	$2.2 \cdot 10^{-4}$
308.4	$2.17 \cdot 10^{-4}$ (T; Ref. 2)	$2.2 \cdot 10^{-4}$
318.4	$2.27 \cdot 10^{-4}$ (T; Ref. 2)	$2.4 \cdot 10^{-4}$

References

[1]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

[2]R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).

Components:
(1) 1,4-Cyclohexadiene; C_6H_8; [628-41-1]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

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

Experimental Data

The solubility of 1,4-cyclohexadiene in water at 25 °C was reported to be 700 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0700 g(1)/100 g sln and $1.57 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 16 mg(1)/kg(2) (standard deviation of mean).

Components:	**Original Measurements:**
(1) 1,4-Cyclohexadiene; C_6H_8; [628-41-1] (2) Water; H_2O; [7732-18-5]	R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).
Variables:	**Prepared By:**
Temperature: 278.26 K–318.36 K	M. C. Haulait-Pirson

Experimental Data

Solubility of 1,4-cyclohexadiene in water

T/K	$10^3 \cdot x_1$	g(1)/100 g sln
278.26	0.1915	0.08519±0.0019
288.36	0.2155	0.09585±0.0028
298.26	0.2105	0.09362±0.0023
308.36	0.2166	0.09634±0.0023
318.36	0.2271	0.10100±0.0023

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Columbia Organic Chemicals Co., Inc.; 99%; used as received.
(2) Laboratory distilled water

Estimated Error:

Solubility: standard deviation from at least 15 measurements are given above.

3.2. Cyclohexene*

Components:	**Evaluators:**
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, July, 2003.

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

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
Budantseva *et al.*[1]	293	McBain and Lissant[6]	298
Duque-Estrada *et al.*[2]	298	Natarajan and Venkatachalam[7]	303
Farkas[4]	298	Pierotti and Liabastre[8]	278–318
McAuliffe[5]	298	Schwarz[9]	297

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

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

where: $\ln x_{1,\min} = -9.83$; $\Delta_{sln}C_p/R = 35.3$; $T_{\min} = 298$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the experimental and reference data are listed in Table 2. The data of Budantseva *et al.*,[1] McAuliffe,[5] Pierotti and Liabastre,[8] and Schwarz[9] are in good agreement with each other and with the reference data (within 30% relative standard deviation) and therefore are Tentative. The data of Duque-Estrada *et al.*,[2] Farkas,[4] McBain and Lissant,[6] and Natarajan and Venkatachalam[7] are in poor agreement with the reference data and are Doubtful.

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

T/K	Experimental values x_1 (T = tentative, D = doubtful)	Reference values x_1 ± 30%
278.3	$6.14 \cdot 10^{-5}$ (T; Ref. 8)	$5.8 \cdot 10^{-5}$
288.4	$6.55 \cdot 10^{-5}$ (T; Ref. 8)	$5.5 \cdot 10^{-5}$
293.2	$5.00 \cdot 10^{-5}$ (T; Ref. 1)	$5.4 \cdot 10^{-5}$
296.7	$6.16 \cdot 10^{-5}$ (T; Ref. 9), $6.27 \cdot 10^{-5}$ (T; Ref. 9)	$5.4 \cdot 10^{-5}$
298.2	$4.67 \cdot 10^{-5}$ (T; Ref. 5), $2.90 \cdot 10^{-5}$ (D; Ref. 6), $3.10 \cdot 10^{-5}$ (D; Ref. 2), $3.50 \cdot 10^{-5}$ (D; Ref. 4)	$5.4 \cdot 10^{-5}$
298.3	$6.56 \cdot 10^{-5}$ (T; Ref. 8)	$5.4 \cdot 10^{-5}$
303.2	$8.91 \cdot 10^{-5}$ (D; Ref. 7)	$5.4 \cdot 10^{-5}$
308.4	$6.63 \cdot 10^{-5}$ (T; Ref. 8)	$5.5 \cdot 10^{-5}$
318.4	$6.81 \cdot 10^{-5}$ (T; Ref. 8)	$5.8 \cdot 10^{-5}$

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

The experimental solubility for (1) in (2) have been investigated by Budantseva *et al.*[1] at 293 K and Englin *et al.*[3] at 283–313 K.

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

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

where: $d_1 = -0.307$; $d_2 = -3.095$; $d_3 = -1.147$; $d_4 = -6.791$; $T_r = T/533.6$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of cyclohexene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 3. The data of Englin *et al.*[3] at 293 K–313 K are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Budantseva *et al.*[1] at 293 K and Englin *et al.*[3] at 283 K are in poor agreement with the reference data and are Doubtful.

TABLE 3. Experimental values for solubility of water (2) in cyclohexene (1)

T/K	Experimental values x_2 (T = tentative, D = doubtful)	Reference values $x_2 \pm 30\%$
283.2	$1.15 \cdot 10^{-3}$ (D; Ref. 3)	$8.1 \cdot 10^{-4}$
293.2	$1.44 \cdot 10^{-3}$ (T; Ref. 3), $1.90 \cdot 10^{-3}$ (D; Ref. 1)	$1.1 \cdot 10^{-3}$
303.2	$1.93 \cdot 10^{-3}$ (T; Ref. 3)	$1.6 \cdot 10^{-3}$
313.2	$2.56 \cdot 10^{-3}$ (T; Ref. 3)	$2.1 \cdot 10^{-3}$

References:

[1] L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).

[2] E. Duque-Estrada, A. H. Bayne, and D. A. Manalan, Instr. Lab. Rept., Dept. Chem. Eng., MIT, April 22 (1964).

[3] B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

[4] E. J. Farkas, Anal. Chem. **37**, 1173 (1965).

[5] C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

[6] J. W. McBain and K. J. Lissant, J. Phys. Colloid Chem. **55**, 665 (1951).

[7] G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).

[8] R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).

[9] F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Components:
(1) Cyclohexene; C_6H_{10}; [110-83-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Data

The solubility of cyclohexene in water at 20 °C was reported to be $x_1 = 5 \cdot 10^{-5}$.

The corresponding mass percent calculated by the compiler is 0.023 $g(1)$/100 g sln.

The solubility of water in cyclohexene at 20 °C was reported to be $x_2 = 0.0019$.

The corresponding mass percent calculated by the compiler is 0.042 $g(2)$/100 g sln.

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components:	Original Measurements:
(1) Cyclohexene; C_6H_{10} ; [110-83-8] (2) Water; H_2O; [7732-18-5]	E. Duque-Estrada, A. H. Bayne, and D. A. Manalan, Instr. Lab. Rept., Dept. Chem. Eng., MIT, April 22 (1964).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of cyclohexene in water at 77 °F was reported to be 0.000107 lb mol(1)/ft^{3}sln.

The corresponding temperature, mass percent, and mole fraction, x_1, values calculated by compilers are 25 °C, 0.014 g(1)/100 g sln, and $3.1 \cdot 10^{-5}$.

The assumption 1 ft^3 sln = 28.32 kg sln was used in the calculation. The data are taken from Farkas[1].

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
The analytical (glc) method was used. Nothing more was reported in Farkas.[1]	(1) Not specified in Farkas.[1] (2) Not specified in Farkas.[1]
	Estimated Error: Not specified in Farkas.[1]

References:

[1]E. J. Farkas, Anal. Chem. **37**, 1173 (1965).

Components:	Original Measurements:
(1) Cyclohexene; C_6H_{10} ; [110-83-8] (2) Water; H_2O; [7732-18-5]	B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
Variables:	**Prepared By:**
Temperature: 10 °C–40 °C	A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in cyclohexene

t/°C	$10^3 \cdot x_2$ (compiler)	G(2)/100 g sln
10	1.15	0.0252
20	1.44	0.0317
30	1.93	0.0424
40	2.56	0.0562

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.	(1) Not specified. (2) Not specified.
	Estimated Error: Not specified.

Components:
(1) Cyclohexene; C_6H_{10} ; [110-83-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. J. Farkas, Anal. Chem. **37**, 1173 (1965).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and A. Szafranski

Experimental Data

The solubility of cyclohexene in water at 77 °F was reported to be 0.000114, 0.000121, and 0.000128 lb mol(1)·/ft^3.

The corresponding temperature, mass percent, and mole fraction, x_1, calculated by compilers at 25 °C, 0.016 g(1)/100 g sln, and $3.5 \cdot 10^{-5}$.

The assumption that 1 ft^3 sln = 28.32 kg sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) has been evaluated from vapor pressure measurements in a specially constructed reactor described in the paper. Theoretical basis is included.

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

Estimated Error:
Solubility: ±6% (mean from three determinations) (compiler).

Components:
(1) Cyclohexene; C_6H_{10} ; [110-83-8]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

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

Experimental Data

The solubility of cyclohexene in water at 25 °C was reported to be 213 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0213 g(1)/100 g sln and $4.67 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum of Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 10 mg(1)/kg(2) (standard deviation of mean).

Components:	Original Measurements:
(1) Cyclohexene; C_6H_{10} ; [110-83-8] (2) Water; H_2O; [7732-18-5]	J. W. McBain and K. J. Lissant, J. Phys. Colloid Chem. **55**, 665 (1951).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson and G. T. Hefter

Experimental Data

The solubility of cyclohexene in water at 25 °C was reported to be 0.013 $g(1)$/100 mL sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers assuming solution density to be the same as pure water (1.00 g/mL), are 0.013 g sln and $2.9 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
10 mL portions of (2) were pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the equilibrium composition.	(1) Eastman No. 1043. (2) Distilled and boiled to remove CO_2. **Estimated Error:** Not specified.

Components:	Original Measurements:
(1) Cyclohexene: C_6H_{10} ; [110-83-8] (2) Water; H_2O; [7732-18-5]	G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).
Variables:	**Prepared By:**
One temperature: 30 °C	M. C. Haulait-Pirson, and G. T. Hefter

Experimental Values

The solubility of cyclohexene in water was reported to be $4.950 \cdot 10^{-3}$ mol/L at 30 °C. (It should be noted that although the authors state that the solubility refers to "water" the context in the paper is ambiguous and the data were probably obtained in 0.001 mol·/L HNO_3 solution.)

Assuming a solution density of 1.00 g/mL the corresponding mass percent and mole fraction (x_1) solubilities calculated by the compilers are respectively, 0.0406 $g(1)$/100 g sln and $8.91 \cdot 10^{-5}$.

Solubility data are also presented as a function of temperature in various salt solutions.

Auxiliary Information

Method/Apparatus/Procedure:	Source and Purity of Materials:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the (1) content determined by titration with bromine using standard procedures.	(1) Prepared by dehydration of cyclohexanol and then washed, dried, and fractioned. Purity (no specification) was determined by chromatography. (2) Not specified. **Estimated Error:** Temperature: ±0.05 °C. Solubility: not specified.

Components:
(1) Cyclohexene; C_6H_{10} ; [110-83-8]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 278.26–318.36 K

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of cyclohexene in water

T/K	$10^3 \cdot x_1$	$g(1)$/100 g sln
278.26	0.06141	0.02800 ± 0.00069
288.36	0.06546	0.02985 ± 0.00061
298.26	0.06557	0.02990 ± 0.00082
308.36	0.6634	0.03025 ± 0.00070
318.36	0.06809	0.03105 ± 0.00093

Auxiliary Information

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

Source and Purity of Materials:
(1) Eastman Organic Chemicals, No. 1043; washed with water to remove stabilizing agent.
(2) Laboratory distilled water.

Estimated Errors:
Solubility: standard deviations from at least 15 measurements are given above.

Components:
(1) Cyclohexene; C_6H_{10} ; [110-83-8]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 23.5 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of cyclohexene in water

t/°C	$10^3 \cdot x_1$ (compiler)	$g(1)$/100 g sln
23.5	6.16	0.0281 ± 0.0005
23.5	6.27	0.0286 ± 0.0013

Auxiliary Information

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

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

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 3% (average standard deviation).

3.3. 1,5-Hexadiene*

Components:
(1) 1,5-Hexadiene; C_6H_{10} ; [592-42-7]
(2) Water; H_2O; [7732-18-5]

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

Critical Evaluation of the Solubility of 1,5-Hexadiene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by McAuliffe[2] at 298 K.

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

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

where: $\ln x_{1,\min} = -9.66$; $\Delta_{sln}C_P/R = 40.1$; $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference data of McAuliffe[2] are listed in Table 4. The data are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

TABLE 4. Experimental values for solubility of 1,5-hexadiene (1) in water (2)

T/K	Experimental values x_1 (D = doubtful)	Reference values $x_1 \pm 30\%$
298.2	$3.70 \cdot 10^{-5}$ (D; Ref. 2)	$6.5 \cdot 10^{-5}$

Critical Evaluation of the Solubility of Water (2) in 1,5-Hexadiene (1)

The experimental solubility for (1) in (2) have been investigated by Black[1] at 286 and 293 K.

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

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

where: $d_1 = -0.989$; $d_2 = -1.624$; $d_3 = 0.876$; $d_4 = -10.836$; $T_r = T/493.8$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1,5-hexadiene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 5. The data of Black[1] at 286 K are in good agreement with the reference data and are Tentative. The data of Black[1] at 293 K are in poor agreement with the reference data and are Doubtful.

TABLE 5. Experimental values for solubility of water (2) in 1,5-hexadiene (1)

T/K	Experimental values x_2 (T = tentative, D = doubtful)	Reference values $x_2 \pm 30\%$
286.2	$2.81 \cdot 10^{-3}$ (T; Ref. 1)	$2.3 \cdot 10^{-3}$
293.2	$4.37 \cdot 10^{-3}$ (D; Ref. 1)	$2.9 \cdot 10^{-3}$

References:
[1]C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).
[2]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

Components:
(1) 1,5-Hexadiene; C_6H_{10} ; [592-42-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 13.5 °C and 20.0 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in 1,5-hexadiene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln	$g(2)$/100 g sln (compiler)
13.5	2.81	0.0618	0.0618
20.2	4.37	0.0969	0.0962

At total saturation pressure of 1 atm.

Auxiliary Information

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

Source and Purity of Materials:
(1) Harvard University; purity not specified; used as received.
(2) Not specified.

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

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

Components:	**Original Measurements:**
(1) 1,5-Hexadiene; C_6H_{10}; [592-42-7] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of 1,5-hexadiene in water at 25 °C was reported to be 169 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0169 g(1)/100 g sln and $3.70 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 6 mg(1)/kg(2) (standard deviation of mean).

3.4. 1-Hexyne*

Components:	**Evaluators:**
(1) 1-Hexyne; C_6H_{10}; [693-02-7] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, July 2003.

Critical Evaluation of the Solubility of 1-Hexyne (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by McAuliffe[1] and Tewari *et al.*[2] at 298 K. Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 1 and expressed by Eq. (1):

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

where: $\ln x_{1,\min} = -9.38$; $\Delta_{sln}C_p/R = 38.6$; $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference data of McAuliffe[1] and Tewari *et al.*[2] are listed in Table 6. The data of McAuliffe[1] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The data of Tewari *et al.*[2] are in poor agreement with the reference data and are Doubtful.

TABLE 6. Experimental values for solubility of 1-hexyne (1) in water (2)

T/K	Experimental values x_1 (T = tentative, D = doubtful)	Reference values $x_1 \pm 30\%$
298.2	$7.89 \cdot 10^{-5}$ (T; Ref. 1), $1.51 \cdot 10^{-4}$ (D; Ref. 2)	$8.6 \cdot 10^{-5}$

References:

[1]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).

[2]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Components:
(1) 1-Hexyne; C_6H_{10}; [693-02-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

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

Experimental Data

The solubility of 1-hexyne in water at 25 °C was reported to be 360 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0360 $g(1)$/100 g sln and $7.89 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:
(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 17 mg(1)/kg(2) (standard deviation of mean).

Components:
(1) 1-Hexyne; C_6H_{10}; [693-02-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of 1-hexyne in water

t/°C	mol(1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$8.37 \cdot 10^{-3}$	$6.90 \cdot 10^{-2}$	$1.512 \cdot 10^{-4}$

Auxiliary Information

Method/Apparatus/Procedure:
A generator column method was used as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with (1) by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by glc method. The column was thermostatted by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

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

Estimated Error:
Temperature: ±0.1 °C
Solubility: 1% (estimated by the authors).

References:
[1]H. De Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

3.5. Cyclohexane*

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

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

Listed below are the experimental solubility data for (1) in (2) which have been investigated by the authors, together with temperature range and pressure range, if reported:

Author (s)	T/K	Author (s)	T/K
Budantseva *et al.*[4]	293	Mackay *et al.*[21]	298
Durand[6]	289	McAuliffe[22]	298
Groves[11]	298	McBain and Lissant[23]	298
Guseva and Parnov[12]	298–494	Pierotti and Liabastre[24]	278–318
Guseva and Parnov[13]	329–494	Price[26]	298
Korenman and Aref'eva[16]	293	Rudakov and Lutsyk[29]	298
Korenman and Aref'eva[17]	298	Sanemasa *et al.*[30]	298
Leinonen and Mackay[19]	298	Schwarz[31]	297
Mackay and Shiu[20]	298	Tsonopoulos *et al.*[35]	313–482 (32–2965 kPa)

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

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

where: $\ln x_{\min,1} = -11.31$; $\Delta_{sln}C_P/R = 36.8$; $T_{min} = 298$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 7. In this and the following tables ⟪good agreement⟫ means that relative standard deviations are within 30%.

The experimental and reference data are listed in Table 8 and shown in Fig. 1. The Recommended and Tentative data are shown in Fig. 2.

TABLE 7. The data categories for solubility of cyclohexane (1) in water (2)

T/K	Recommended (data in good agreement with each other and with the reference data)	Tentative (data in good agreement with the reference data)	Doubtful (data in poor agreement with the reference data)
278.3		Pierotti and Liabastre[24]	
288.4			Pierotti and Liabastre[24]
289.2		Durand[6]	
293.2		Budantseva *et al.*[4]	Korenman and Aref'eva[16]
296.7		Schwarz[31]	
298.2	Groves[11] Leinonen and Mackay[19] Mackay and Shiu[20] Mackay *et al.*[21] McAuliffe[22] Price[26] Rudakov and Lutsyk[29] Sanemasa *et al.*[30]	Guseva and Parnov[12] McBain and Lissant[23]	Korenman and Aref'eva[17]
298.3			Pierotti and Liabastre[24]
308.4			Pierotti and Liabastre[24]
313.2		Tsonopoulos *et al.*[35]	
318.4			Pierotti and Liabastre[24]
329.2			Guseva and Parnov[12,13]
367.2			Guseva and Parnov[12,13]
373.2		Tsonopoulos *et al.*[35]	
400.2			Guseva and Parnov[12,13]
422.0		Tsonopoulos *et al.*[35]	
423.2		Tsonopoulos *et al.*[35]	
435.2			Guseva and Parnov[12,13]
473.2		Tsonopoulos *et al.*[35]	
482.2		Tsonopoulos *et al.*[35]	
493.7			Guseva and Parnov[12,13]

TABLE 8. Experimental values for solubility of cyclohexane (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
278.3		$1.84 \cdot 10^{-5}$ (T; Ref. 24)	$1.5 \cdot 10^{-5}$
288.4		$1.99 \cdot 10^{-5}$ (D; Ref. 24)	$1.4 \cdot 10^{-5}$
289.2		$1.30 \cdot 10^{-5}$ (T; Ref. 6)	$1.4 \cdot 10^{-5}$
293.2		$1.50 \cdot 10^{-5}$ (T; Ref. 4), $2.10 \cdot 10^{-5}$ (D; Ref. 16)	$1.3 \cdot 10^{-5}$
296.7		$1.10 \cdot 10^{-5}$ T; (Ref. 31)	$1.3 \cdot 10^{-5}$
298.2		$1.25 \cdot 10^{-5}$ (R; Ref. 11), $1.70 \cdot 10^{-5}$ (T; Ref. 12), $2.60 \cdot 10^{-5}$ (D; Ref. 17), $1.21 \cdot 10^{-5}$ (R; Ref. 19), $1.23 \cdot 10^{-5}$ (R; Ref. 20), $1.20 \cdot 10^{-5}$ (R; Ref. 21), $1.18 \cdot 10^{-5}$ (R; Ref. 22), $1.70 \cdot 10^{-5}$ (T; Ref. 23), $1.42 \cdot 10^{-5}$ (R; Ref. 26), $1.20 \cdot 10^{-5}$ (R; Ref. 29), $1.13 \cdot 10^{-5}$ (R; Ref. 30)	$1.3 \cdot 10^{-5}$
298.3		$2.00 \cdot 10^{-5}$ (D; Ref. 24)	$1.3 \cdot 10^{-5}$
308.4		$2.00 \cdot 10^{-5}$ (D; Ref. 24)	$1.4 \cdot 10^{-5}$
313.2	31.51 (Ref. 35)	$1.56 \cdot 10^{-5}$ (T; Ref. 35)	$1.4 \cdot 10^{-5}$
318.4		$2.07 \cdot 10^{-5}$ (D; Ref. 24)	$1.4 \cdot 10^{-5}$
329.2		$3.60 \cdot 10^{-5}$ (D; Ref. 12), $3.06 \cdot 10^{-5}$ (D; Ref. 13)	$1.6 \cdot 10^{-5}$
367.2		$6.00 \cdot 10^{-5}$ (D; Ref. 12), $5.06 \cdot 10^{-5}$ (D; Ref. 13)	$2.8 \cdot 10^{-5}$
373.2	272.3 (Ref. 35)	$3.79 \cdot 10^{-5}$ (T; Ref. 35)	$3.2 \cdot 10^{-5}$
400.2		$1.11 \cdot 10^{-4}$ (D; Ref. 12), $1.01 \cdot 10^{-4}$ (D; Ref. 13)	$5.7 \cdot 10^{-5}$
422.0		$1.03 \cdot 10^{-4}$ (T; Ref. 35)	$9.8 \cdot 10^{-5}$
423.2	1003.2 (Ref. 35)	$1.30 \cdot 10^{-4}$ (T; Ref. 35)	$1.0 \cdot 10^{-4}$
435.2		$3.13 \cdot 10^{-4}$ (D; Ref. 12), $3.01 \cdot 10^{-4}$ (D; Ref. 13)	$1.4 \cdot 10^{-4}$
473.2	2965 (Ref. 35)	$3.92 \cdot 10^{-4}$ (T; Ref. 35)	$4.0 \cdot 10^{-4}$
482.2		$4.93 \cdot 10^{-4}$ (T; Ref. 35)	$5.1 \cdot 10^{-4}$
493.7		$3.87 \cdot 10^{-3}$ (D; Ref. 12), $3.78 \cdot 10^{-3}$ (D; Ref. 13)	$7.1 \cdot 10^{-4}$

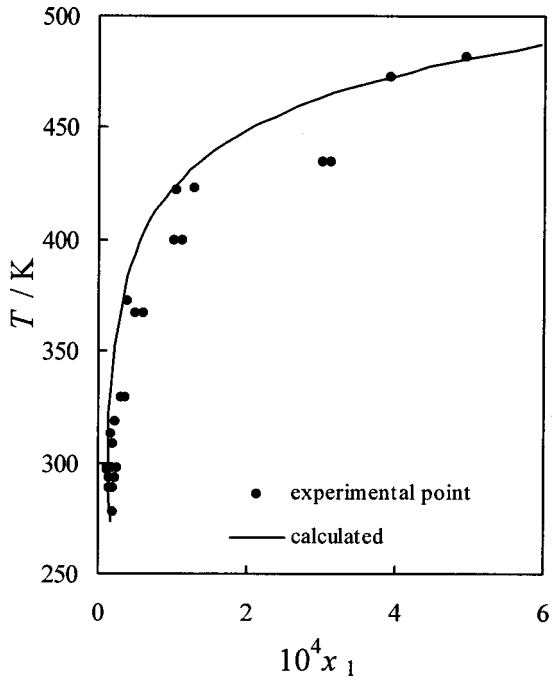

FIG. 1. All the solubility data for cyclohexane (1) in water (2).

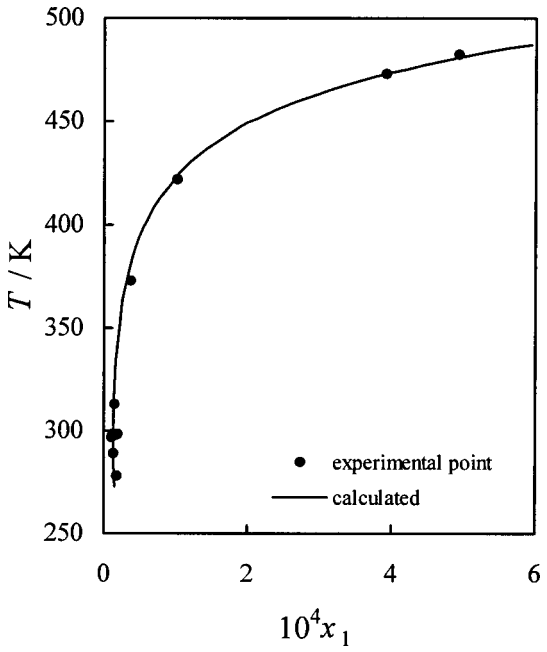

FIG. 2. Recommended and tentative solubility data for cyclohexane (1) in water (2).

Critical Evaluation of the Solubility of Water (2) Cyclohexane (1)

The experimental solubility data for (2) in (1) have been investigated by the authors listed below together with temperature range and pressure range, if reported:

Author (s)	T/K	Author (s)	T/K
Berkengeim[1]	293 and 323	Johnson *et al.*[14]	298
Black *et al.*[2]	293	Kirchnerova and Cave[15]	298
Budantseva *et al.*[4]	293	Plenkina *et al.*[25]	403–523
Burd and Braun[5]	368–478 (172–3103 kPa)	Roddy and Coleman[28]	298
Englin *et al.*[7]	283–323	Stephenson[33]	313
Glasoe and Schultz[8]	288–303	Tarassenkow and Poloshinzewa[34]	287–326
Goldman[9]	283–313	Tsonopoulos *et al.*[35]	313–482 (32–2965 kPa)
Gregory *et al.*[10]	298	Zel'venskii *et al.*[36]	293

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

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

where: $d_1 = -0.963$; $d_2 = -6.267$; $d_3 = -0.710$; $d_4 = -3.111$; $T_r = T/533.3$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of cyclohexane in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories listed in Table 9.

The experimental and reference solubility data for (2) in (1) are listed in Table 10 and shown in Fig. 3. The Recommended and Tentative data are shown in Fig. 4.

TABLE 9. The data categories for solubility of water (2) in cyclohexane (1)

T/K	Recommended (data in good agreement with each other and with the reference data)	Tentative (data in good agreement with the reference data)	Doubtful (data in poor agreement with the reference data)
283.2		Goldman[9]	Englin *et al.*[7]
287.2		Tarassenkow and Poloshinzewa[34]	
288.2		Glasoe and Schultz,[8] Goldman[9]	
292.2			Tarassenkow and Poloshinzewa[34]
293.2		Berkengeim,[1] Goldman[9]	Black *et al.*[2] Budantseva *et al.*[4] Englin *et al.*[7] Tarassenkow and Poloshinzewa[34] Zel'venskii *et al.*[36]
298.2	Glasoe and Schultz[8] Goldman[9] Gregory *et al.*[10] Kirchnerova and Cave[15] Roddy and Coleman[28]		Johnson *et al.*[14]
301.7			Tarassenkow and Poloshinzewa[34]
303.2	Glasoe and Schultz[8] Goldman[9]		Englin *et al.*[7]
305.7			Tarassenkow and Poloshinzewa[34]
308.2		Goldman[9]	
311.2			Tarassenkow and Poloshinzewa[34]
313.2		Goldman,[9] Tsonopoulos *et al.*[35]	Englin *et al.*[7] Stephenson[33] Tsonopoulos *et al.*[35]
323.2			Berkengeim[1] Englin *et al.*[7]
326.2			Tarassenkow and Poloshinzewa[34]
366.5			Burd and Braun[5]
367.6			Burd and Braun[5]
373.2		Tsonopoulos *et al.*[35]	Tsonopoulos *et al.*[35]
389.3			Burd and Braun[5]
394.3			Burd and Braun[5]
403.2			Plenkina *et al.*[25]
413.2			Burd and Braun[5]
422.0			Burd and Braun[5]
423.2		Tsonopoulos *et al.*[35]	
428.7			Burd and Braun[5]
436.2			Plenkina *et al.*[25]
440.4			Burd and Braun[5]
449.8			Burd and Braun[5]
450.8			Burd and Braun[5]
457.6			Burd and Braun[5]
464.8			Burd and Braun[5]
470.9			Burd and Braun[5]
461.2			Plenkina *et al.*[25]
473.2		Tsonopoulos *et al.*[35]	
477.6			Burd and Braun[5]
474.0			Plenkina *et al.*[25]
486.7			Plenkina *et al.*[25]
492.2			Plenkina *et al.*[25]
505.2			Plenkina *et al.*[25]
517.2			Plenkina *et al.*[25]
523.2			Plenkina *et al.*[25]

TABLE 10. Experimental values for solubility of water (2) in cyclohexane (1)

T/K	P/kPa	Experimental values x_2 (R=recommended, T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
283.2		$3.10\cdot10^{-4}$ (D; Ref. 7), $1.60\cdot10^{-4}$ (T; Ref. 9)	$2.0\cdot10^{-4}$
287.2		$2.30\cdot10^{-4}$ (T; Ref. 34)	$2.4\cdot10^{-4}$
288.2		$2.80\cdot10^{-4}$ (T; Ref. 8), $2.00\cdot10^{-4}$ (T; Ref. 9)	$2.6\cdot10^{-4}$
292.2		$4.70\cdot10^{-4}$ (D; Ref. 34)	$3.1\cdot10^{-4}$
293.2		$4.10\cdot10^{-4}$ (T; Ref. 1), $4.70\cdot10^{-4}$ (D; Ref. 2), $4.70\cdot10^{-4}$ (D; Ref. 4), $5.70\cdot10^{-4}$ (D; Ref. 7), $2.80\cdot10^{-4}$ (T; Ref. 9), $4.70\cdot10^{-4}$ (D; Ref. 34), $4.60\cdot10^{-4}$ (D; Ref. 36)	$3.2\cdot10^{-4}$
298.2		$3.50\cdot10^{-4}$ (R; Ref. 8), $3.30\cdot10^{-4}$ (R; Ref. 9), $3.20\cdot10^{-4}$ (R; Ref. 10), $2.60\cdot10^{-4}$ (D; Ref. 14), $3.30\cdot10^{-4}$ (R; Ref. 15), $3.75\cdot10^{-4}$ (R; Ref. 28)	$4.0\cdot10^{-4}$
301.7		$7.00\cdot10^{-4}$ (D; Ref. 34)	$4.7\cdot10^{-4}$
303.2		$9.06\cdot10^{-4}$ (D; Ref. 7), $4.10\cdot10^{-4}$ (R; Ref. 8), $4.50\cdot10^{-4}$ (R; Ref. 9)	$5.0\cdot10^{-4}$
305.7		$9.30\cdot10^{-4}$ (D; Ref. 34)	$5.6\cdot10^{-4}$
308.2		$5.30\cdot10^{-4}$ (T; Ref. 9)	$6.2\cdot10^{-4}$
311.2		$1.45\cdot10^{-3}$ (D; Ref. 34)	$7.0\cdot10^{-4}$
313.2	31.51 (Ref. 35)	$1.48\cdot10^{-3}$ (D; Ref. 7), $6.10\cdot10^{-4}$ (T; Ref. 9), $2.80\cdot10^{-4}$ (D; Ref. 33), $9.24\cdot10^{-4}$ (T; Ref. 35), $8.87\cdot10^{-4}$ (T; Ref. 35), $1.13\cdot10^{-3}$ (D; Ref. 35)	$7.6\cdot10^{-4}$
323.2		$7.00\cdot10^{-4}$ (D; Ref. 1), $2.29\cdot10^{-3}$ (D; Ref. 7)	$1.1\cdot10^{-3}$
326.2		$2.33\cdot10^{-3}$ (D; Ref. 34)	$1.3\cdot10^{-3}$
366.5	165 (Ref. 5)	$1.02\cdot10^{-2}$ (D; Ref. 5)	$5.1\cdot10^{-3}$
367.6	172 (Ref. 5)	$1.02\cdot10^{-2}$ (D; Ref. 5)	$5.3\cdot10^{-3}$
373.2	272.3 (Ref. 35)	$4.35\cdot10^{-3}$ (T; Ref. 35), $5.12\cdot10^{-3}$ (T; Ref. 35)	$6.3\cdot10^{-3}$
389.3	345 (Ref. 5)	$2.11\cdot10^{-2}$ (D; Ref. 5)	$1.0\cdot10^{-2}$
394.3	407 (Ref. 5)	$2.25\cdot10^{-2}$ (D; Ref. 5)	$1.2\cdot10^{-2}$
403.2		$3.60\cdot10^{-2}$ (D; Ref. 25)	$1.5\cdot10^{-2}$
413.2	689 (Ref. 5)	$3.72\cdot10^{-2}$ (D; Ref. 5)	$2.0\cdot10^{-2}$
422.0	876 (Ref. 5)	$4.64\cdot10^{-2}$ (D; Ref. 5)	$2.5\cdot10^{-2}$
423.2	1008.2 (Ref. 35)	$2.04\cdot10^{-2}$ (T; Ref. 35), $2.40\cdot10^{-2}$ (T; Ref. 35)	$2.6\cdot10^{-2}$
428.7	1034 (Ref. 5)	$5.37\cdot10^{-2}$ (D; Ref. 5)	$3.0\cdot10^{-2}$
436.2		$9.30\cdot10^{-2}$ (D; Ref. 25)	$3.6\cdot10^{-2}$
440.4	1379 (Ref. 5)	$6.98\cdot10^{-2}$ (D; Ref. 5)	$4.0\cdot10^{-2}$
449.8	1724 (Ref. 5)	$8.42\cdot10^{-2}$ (D; Ref. 5)	$5.0\cdot10^{-2}$
450.8	1724 (Ref. 5)	$8.30\cdot10^{-2}$ (D; Ref. 5)	$5.1\cdot10^{-2}$
457.6	2068 (Ref. 5)	$9.71\cdot10^{-2}$ (D; Ref. 5)	$6.0\cdot10^{-2}$
461.2		$1.30\cdot10^{-1}$ (D; Ref. 25)	$6.5\cdot10^{-2}$
464.8	2413 (Ref. 5)	$1.109\cdot10^{-1}$ (D; Ref. 5)	$7.1\cdot10^{-2}$
470.9	2758 (Ref. 5)	$1.262\cdot10^{-1}$ (D; Ref. 5)	$8.2\cdot10^{-2}$
473.2	2965 (Ref. 35)	$7.93\cdot10^{-2}$ (T; Ref. 35)	$8.6\cdot10^{-2}$
474.0		$1.54\cdot10^{-1}$ (D; Ref. 25)	$8.8\cdot10^{-2}$
477.6	3103 (Ref. 5)	$1.52\cdot10^{-1}$ (D; Ref. 5)	$9.5\cdot10^{-2}$
486.7		$1.93\cdot10^{-1}$ (D; Ref. 25)	$1.2\cdot10^{-1}$
492.2		$2.16\cdot10^{-1}$ (D; Ref. 25)	$1.3\cdot10^{-1}$
505.2		$2.65\cdot10^{-1}$ (D; Ref. 25)	$1.8\cdot10^{-1}$
517.2		$3.22\cdot10^{-1}$ (D; Ref. 25)	$2.3\cdot10^{-1}$
523.2		$3.50\cdot10^{-1}$ (D; Ref. 25)	$2.7\cdot10^{-1}$

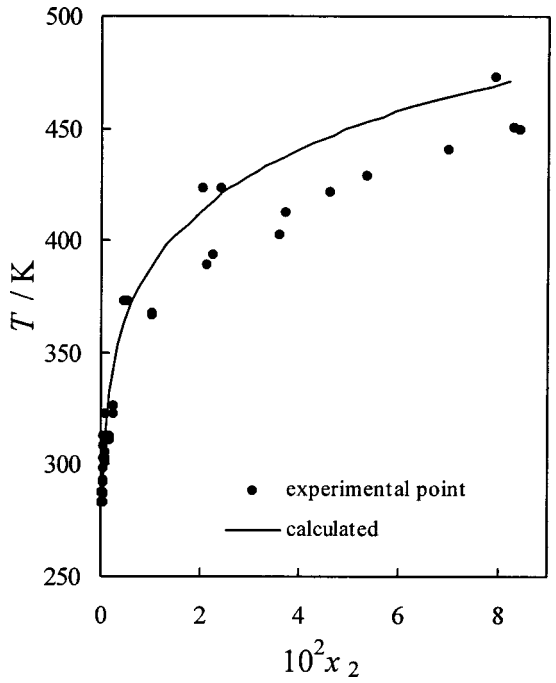

FIG. 3. All the solubility data for water (2) in cyclohexane (1).

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[40] are independent data. The data reported by Hayworth,[38] Hicks and Young,[39] Roof,[41] Scott and van Konynenburg,[42] lack sufficient information to justify evaluation. Therefore these data are Rejected. The publications of Bennet and Philip,[37] Sultanov and Skripka[43] were not accesible for compilers.

References:

[1]T. I. Berkengeim, Zavod. Lab. **10**, 592 (1941).
[2]C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).
[3]K. Bröllos, K. Peter, and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **74**, 682 (1970).
[4]L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).
[5]S. D. Burd, Jr. and W. G. Braun, Proc. Am. Pet. Inst., Div. Refin. **48**, 464 (1968).
[6]R. Durand, C. R. Acad. Sci. **226**, 409 (1948).
[7]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[8]P. K. Glasoe and S. D. Schultz, J. Chem. Eng. Data **17**, 66 (1972).
[9]S. Goldman, Can. J. Chem. **52**, 1668 (1974).
[10]M. D. Gregory, S. D. Christian, and H. E. Affsprung, J. Phys. Chem. **71**, 2283 (1967).
[11]F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).
[12]A. N. Guseva and E. I. Parnov, Zh. Fiz. Khim. **37**, 2763 (1963).
[13]A. N. Guseva and E. I. Parnov, Radiokhimiya **5**, 507 (1963).
[14]J. R. Johnson, S. D. Christian, and H. E. Affsprung, J. Chem. Soc. A, 77 (1966).
[15]J. Kirchnerova and G. C. B. Cave, Can. J. Chem. **54**, 3909 (1976).
[16]I. M. Korenman and R. P. Aref'eva, Patent USSR, 553 524, 1977.04.057
[17]I. M. Korenman and R. P. Aref'eva, Zh. Prikl. Khim. (Leningrad) **51**, 957 (1978).
[18]A. P. Kudchadker and J. J. McKetta, AIChE J. **7**, 707 (1961).
[19]P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. **51**, 230 (1973).
[20]D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. **53**, 239 (1975).
[21]D. Mackay, W. J. Shiu, and A. W. Wolkoff, ASTM Spec. Tech. Pub. **573**, 251 (1975).

Components:	**Original Measurements:**
(1) Cyclohexane; C_6H_{12} ; [110-82-7] (2) Water; H_2O; [7732-18-5]	T. I. Berkengeim, Zavod. Lab. **10**, 592 (1941).
Variables:	**Prepared By:**
Temperature: 20 °C and 50 °C	A. Maczynski

Experimental Data

Solubility of water in cyclohexane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
20	4.1	0.0087
50	7.0	0.015

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (2) in (1) was determined by the Karl Fischer reagent method.

Source and Purity of Materials:

(1) Source not specified; CP reagent; boiling point 80 °C; used as received.
(2) Not specified.

Estimated Error:

Not specified.

[22]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[23]J. W. McBain and K. J. Lissant, J. Phys. Colloid Chem. **55**, 665 (1951).
[24]R. A. Pierotti and A. A. Liabastre, U.S. NTIS, PB Rep., No 21163, 113 pp (1972).
[25]R. M. Plenkina, R. O. Pryanikova, and G. D. Efremova, Zh. Fiz. Khim. **45**, 2389 (1971).
[26]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[27]C. J. Rebert and K. E. Hayworth, AIChE J. **13**, 118 (1967).
[28]J. W. Roddy and C. F. Coleman, Talanta **15**, 1281 (1968).
[29]E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).
[30]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).
[31]F. P. Schwarz, Anal. Chem. **52**, 10 (1980).
[32]V. G. Skripka, Tr., Vses. Neftegazov. Nauch.-Issled. Inst. **61**, 139 (1976).
[33]R. M. Stephenson, J. Chem. Eng. Data **37**, 80 (1992).
[34]D. N. Tarassenkow and E. N. Poloshinzewa, Ber. Dtsch. Chem. Ges. **65**, 184 (1932).
[35]C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[36]Ya. D. Zel'venskii, A. A. Efremov, and G. M. Larin, Khim. Tekhnol. Topl. Masel **10**, 3 (1965).
[37]G. M. Bennet and W. G. Philip, J. Chem. Soc. 1937 (1928).
[38]K. E. Hayworth, M. S. Thesis, Univ. Southern California, Los Angeles, USA, 1962.
[39]C. P. Hicks and C. L. Young, Chem. Rev. **75**, 119 (1975).
[40]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).
[41]J. G. Roof, J. Chem. Eng. Data **15**, 301 (1970).
[42]R. L. Scott and P. H. van Konynenburg, Phil. Trans. Roy. Soc., London A **298**, 495 (1980).
[43]R. G. Sultanov and V. E. Skripka, Zh. Fiz. Khim. **47**, 1035 (1973); Deposited doc. 1970; VINITI 5347-73.

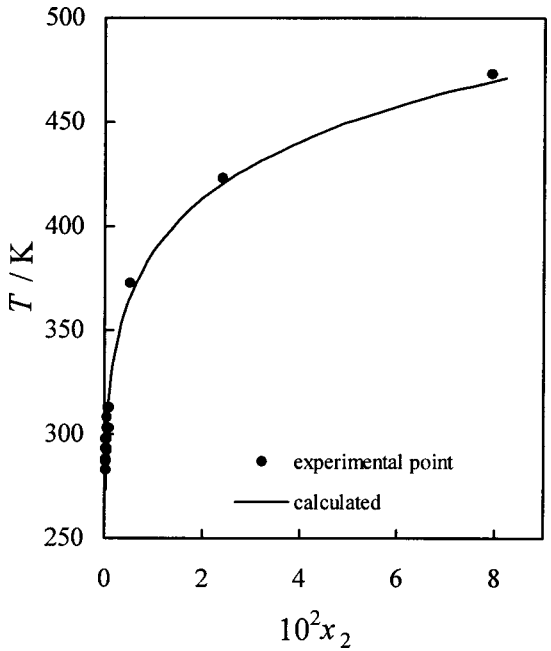

FIG. 4. Recommended and tentative solubility data for water (2) in cyclohexane (1).

Components:	**Original Measurements:**
(1) Cyclohexane; C_6H_{12} ; [110-82-7] (2) Water; H_2O; [7732-18-5]	C. Black, G. G. Joris, and H. S. Taylor, J. Chem. Phys. **16**, 537 (1948).
Variables:	**Prepared By:**
One temperature: 20 °C	M. C. Haulait-Pirson

Experimental Data

The solubility of water in cyclohexane at 20 °C and at a total saturation pressure of 1 atm was reported to be 0.010 $g(2)$/100 g(1). The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.010 $g(2)$/100 g sln and $4.7 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:

The method described by Joris and Taylor[1] in which tritium oxide acts as a tracer, was used.
Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.

Source and Purity of Materials:

(1) Ohio State University under an American Petroleum Institute project; purity not specified; used as received.
(2) Not specified.

Estimated Error:

Solubility: a few percent (type of error not specified).

References:

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

Components:	**Original Measurements:**
(1) Cyclohexane; C_6H_{12} ; [110-82-7] (2) Water; H_2O; [7732-18-5]	K. Bröllos, K. Peter, and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **74**, 682 (1970).
Variables:	**Prepared By:**
Pressure and temperature on one phase-two phase boundary	C. L. Young

Experimental Data

Values of pressure and temperature on the one phase-two phase boundary

T/K	x_1	$g(1)$/100 g sln (compiler)	P/bar
379.8	0.100	34.1	1742
369.0	0.100		1403
363.0	0.100		1200
360.1	0.100		1000
351.5	0.100		798
343.5	0.100		595
333.7	0.100		395
329.2	0.100		328
330.0	0.100		293
333.0	0.100		271
334.2	0.100		245
338.0	0.100		217
392.2	0.150	45.2	1600
384.0	0.150		1400
376.5	0.150		1202
369.2	0.150		1000
361.2	0.150		800
351.0	0.150		600
346.5	0.150		500
340.0	0.150		394
338.0	0.150		347
339.0	0.150		299
340.5	0.150		250
357.7	0.150		222
403.5	0.200	53.9	1610
393.9	0.200		1408
387.0	0.200		1204
378.7	0.200		1002
369.0	0.200		800
359.5	0.200		600
352.2	0.200		500
347.0	0.200		416
343.0	0.200		328
342.0	0.200		298
345.0	0.200		246
355.0	0.200		223
412.4	0.298	66.5	1600
404.7	0.298		1400
396.2	0.298		1200
387.1	0.298		1004
375.3	0.298		800
363.8	0.298		600
360.4	0.298		550

337.5	0.800		600
316.5	0.800		400
305.0	0.800		295
295.1	0.800		244
275.2	0.800		200

Auxiliary Information

Method/Apparatus/Procedure:

Measurements were made in a steel optical cell within an aluminum block furnace. The cell contents were stirred magnetically. Pressure was measured using a movable piston and Bourdon gauge. Temperature was measured with a steel-sheathed thermocouple. Components were charged into the cell and the transition from one phase to two phases was observed visually.

Source and Purity of Materials:

(1) Merck sample purity 99.9 mole %.
(2) Twice distilled.

Estimated Error:

Temperature: $\Delta T/\mathrm{K} = \pm 0.1$.
Pressure: $\Delta P/P = \pm 0.01$ (estimated by compiler).

349.2	0.298		398
346.2	0.298		339
346.5	0.298		237
349.5	0.298		224
352.7	0.298		214
414.9	0.400	75.7	1600
406.5	0.400		1398
399.2	0.400		1200
390.1	0.400		995
378.0	0.400		800
364.3	0.400		600
355.6	0.400		465
347.6	0.400		352
345.0	0.400		295
342.0	0.400		230
335.0	0.400		195
421.5	0.500	82.4	1718
419.0	0.500		1645
416.5	0.500		1584
408.0	0.500		1406
399.0	0.500		1195
388.9	0.500		1004
376.0	0.500		789
364.0	0.500		600
350.0	0.500		460
340.1	0.500		375
343.0	0.500		330
338.5	0.500		250
330.0	0.500		200
413.0	0.600	87.5	1603
405.4	0.600		1405
395.8	0.600		1200
386.4	0.600		1000
375.3	0.600		800
362.0	0.600		595
345.7	0.600		395
336.2	0.600		319
333.4	0.600		290
329.4	0.600		261
326.5	0.600		243
323.1	0.600		220
318.5	0.600		205
406.7	0.700	91.6	1600
399.0	0.700		1405
389.1	0.700		1200
380.5	0.700		1000
367.2	0.700		800
351.1	0.700		588
332.5	0.700		400
325.0	0.700		342
314.0	0.700		299
300.5	0.700		250
395.4	0.800	96.9	1605
387.1	0.800		1403
377.6	0.800		1200
367.2	0.800		1005
353.9	0.800		800

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Data

The solubility of cyclohexane in water at 20 °C was reported to be $x_1 = 1.5 \cdot 10^{-5}$.
The corresponding mass percent calculated by the compiler is 0.0070 $g(1)$/100 g sln.
The solubility of water in cyclohexane at 20 °C was reported to be $x_2 = 4.7 \cdot 10^{-4}$.
The corresponding mass percent calculated by the compiler is 0.0101 $g(2)$/100 g sln.

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature and Pressure

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Hydrocarbon-rich liquid phase composition for the three-phase conditions

t/°F	T/K (compiler)	x_2 (compiler)	$g(2)$/100 g sln	P/psia	P/MPa (compiler)
202	367.59	0.0102	0.22	25	0.172
241	389.26	0.0211	0.46	50	0.345
284	413.15	0.0372	0.82	100	0.689
312	428.70	0.0537	1.20	150	1.034
333	440.37	0.0698	1.58	200	1.379
350	449.81	0.0842	1.93	250	1.724
364	457.60	0.0971	2.25	300	2.068
377	464.82	0.1109	2.60	350	2.413
388	470.93	0.1262	3.00	400	2.758
200	366.48	0.0102	0.22	24	0.165
250	394.26	0.0225	0.49	59	0.407
300	422.04	0.0464	1.03	127	0.876
350	450.82	0.0830	1.90	250	1.724
400	477.60	0.1520	3.70	450	3.103

Auxiliary Information

Method/Apparatus/Procedure:
The vapor and liquid phase compositions have been determined for the (1)–(2) system in the two-phase hydrocarbon-rich liquid region. Equilibrium points were obtained by incremental addition of water followed by stirring, settling, sampling, and chromatographic analysis. This procedure was continued until addition of water resulted in no pressure increase. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Company; 99.5% purity.
(2) Laboratory distilled.

Estimated Error:
Solubility: ±0.004 weight fraction of (2) present.

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 16 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of cyclohexane in water at 16 °C was reported to be 0.08 mL(1)/L(2).

With the assumption of a solution density of 1.00 g/mL and a density value of 0.782 g/mL for cyclohexane at 16 °C (Timmermans[2]), the corresponding mass percent is 0.0062 $g(1)$/100 g sln and the corresponding mole fraction, x_1, is $1.3 \cdot 10^{-5}$ (compiler).

Auxiliary Information

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

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

Estimated Error:
Solubility: ±0.005 mL(1)/L(2).

References:
[1]R. Durand, C. R. Hebd. Seances Acad. Sci. **223**, 898 (1946).
[2]J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 10 °C–50 °C

Prepared By:
A. Maczynski and M. C. Haulait-Pirson

Experimental Data

Solubility of water in cyclohexane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.1	0.0067
20	5.70	0.0122
30	9.06	0.0194
40	14.8	0.0317
50	22.9	0.0490

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. K. Glasoe and S. D. Schultz, J. Chem. Eng. Data **17**, 66 (1972).

Variables:
Temperature: 15 °C–30 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of water in cyclohexane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln (compiler)	mol(2)/L sln
15	2.8	0.0060[a]	0.0026 ± 0.0001
25	3.5	0.0074[a]	0.0032 ± 0.0002
30	4.1	0.0087[a]	0.0037 ± 0.0002

[a]Calculated with the assumption of a solution density of 0.7831, 0.7739, and 0.7692g/mL at, respectively, 15, 25, and 30 °C; these values are the density values of the pure cyclohexane at these temperatures (Timmermans[1]).

Auxiliary Information

Method/Apparatus/Procedure:
(1) was saturated with (2) by allowing it to stand in contact with (2) in a closed pyrex storage bottle protected from atmospheric moisture and placed in a constant temperature water bath. The concentration of (2) in (1) was determined by the Karl Fischer method using a conventional dead-stop end-point apparatus. The Karl Fischer reagent was standardized against sodium tartrate.

Source and Purity of Materials:
(1) Source not specified; reagent grade; purified by distillation and dried over molecular sieve.
(2) Distilled in a pyrex system.

Estimated Error:
Solubility: see above (type of error not specified).

References:
[1]J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 10 °C–40 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of water in cyclohexane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln[a] (compiler)	mol(2)/L sln
10	1.6	0.0034	0.00147
15	2.0	0.0043	0.00185
20	2.8	0.0059	0.00255
25	3.3	0.0070	0.00301
30	4.5	0.0096	0.00410
35	5.3	0.0114	0.00485
40	6.1	0.0131	0.00552

[a]Calculated with the assumption of a solution density of 0.7878, 0.7831, 0.7785, 0.7739, 0.7692, 0.7643, and 0.7595 g/mL, at respectively, 10, 15, 20, 25, 30, 35, and 45 °C; these values are the density values of the pure cyclohexane at these temperatures.[1]

Auxiliary Information

Method/Apparatus/Procedure:
(1) was equilibrated with an excess of (2) in 175 mL bottles fitted with Bakelite screw caps. The bottles immersed in a water bath were given end-over-end rotation at 20 rpm. After equilibration, aliquots (5 mL ± 0.2%) were taken with calibrated Hamilton syringes and injected into the titration vessel. Analyses were performed with an Aquatest II automatic Karl Fischer Titrator.

Source and Purity of Materials:
(1) Certified grade; washed with water, dried with silica gel, and distilled; d (25 °C,4 °C) 0.77390 ± 0.00002.
(2) Distilled.

Estimated Error:
Temperature: ± 0.02 K.
Solubility: ± 0.00024 (mean of standard deviation).

References:
[1]J. Timmermans, *Physico-Chemical Constants of Pure Organic Compounds* (Elsevier, New York, 1950).

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of water in cyclohexane at 25 °C was reported to be 0.00297 mol(2)/L sln.

With the assumption of a solution density of 0.7739 g/mL (density value of pure cyclohexane reported in Goldman[2]), the corresponding mass percent is 0.0069 $g(2)$/100 g sln and the corresponding mole fraction, x_2, is $3.2 \cdot 10^{-4}$ (compiler).

Auxiliary Information

Method/Apparatus/Procedure:
Solubility of (2) in (1) was obtained using the solute isopiestic method described in Christian *et al.*[1] The samples were titrated by the Karl Fischer method using a Beckman KF-3 aquameter. The Karl Fischer reagent was standardized alternatively by titrating weighed amounts of sodium tartrate dihydrate or by titrating a 25 °C water-saturated benzene solution.

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

Estimated Error:
Temperature: ±0.1 °C.

References:
[1]S. D. Christian, H. E. Affsprung, J. R. Johnson, and J. D. Worley, J. Chem. Educ. **40**, 419 (1963).
[2]S. Goldman, Can. J. Chem. **52**, 1668 (1974).

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. R. Groves, J. Chem. Eng. Data **33**, 136 (1988).

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of cyclohexane in water

t/°C	mg(1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	58.4±1.0	0.00586	$1.254 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method, similar to Polak and Liu,[1] was used. Hydrocarbon (1) was injected into a 40 mL vials fitted with Teflon-lined septa containing about 20 mL water and placed in a thermostatted bath for 2 weeks. The water layer was analyzed chromatographically (3% SP-1500 on Carbopack B at 150 °C, He carrier gas at 30 mL/min, FID detector). The reported result is average of four replicate determinations.

Source and Purity of Materials:
(1) Aldrich, Chemical Co.; purity 99.9%; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: as above.

References:
[1]J. Polak and B. C. Y. Liu, Can. J. Chem. **51**, 4018 (1973).

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Zh. Fiz. Khim. **37**, 2763 (1963).

Variables:
Temperature: 25–220.5 °C

Prepared By:
A. Maczynski

Experimental Data

Solubility of cyclohexane in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g sln
25	0.17	0.008
56	0.36	0.017
94	0.60	0.028
127	1.11	0.0517
162	3.13	0.146
220.5	38.72	1.784

The same data is reported in Guseva and Parnov.[1]

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined in sealed glass ampoules at pressures less than 17 kg/cm^2. No more details were reported in the paper.

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

Estimated Error:
Not specified.

References:
[1]A. N. Guseva and E. I. Parnov, Radiokhimiya **5**, 507 (1963).

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of water in cyclohexane at 25 °C was reported to be 0.0024 mol(2)/L sln.

With the assumption of a solution density of 0.7739 g/mL (density value of pure cyclohexane reported in Goldman[2]), the corresponding mass percent is 0.0056 $g(2)$/100 g sln and the corresponding mole fraction, x_2, is $2.6 \cdot 10^{-4}$ (compiler).

Auxiliary Information

Method/Apparatus/Procedure:
The solute isopiestic apparatus described in Christian *et al.*[1] was used. Samples were equilibrated in constant-temperature water baths. Water solubilities were determined using the Beckman Model KF-3 Aquameter.

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

Estimated Error:
Temperature: ±0.1 °C.
Solubility: ±0.0003 mol(2)/L sln (type of error not specified).

References:
[1]S. D. Christian, H. E. Affsprung, J. R. Johnson, and J. D. Worley, J. Chem. Educ. **40**, 419 (1963).
[2]S. Goldman, Can. J. Chem. **52**, 1668 (1974).

Components:	Original Measurements:
(1) Cyclohexane; C_6H_{12} ; [110-82-7] (2) Water; H_2O; [7732-18-5]	J. Kirchnerova and G. C. B. Cave, Can. J. Chem. **54**, 3909 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Data

The solubility of water in cyclohexane at 25 °C was reported to be 0.0030 mol(2)/L sln.

With the assumption of a solution density of 0.7739 g/mL (density value of pure cyclohexane reported in Goldman[1]), the corresponding mass percent is 0.0070 $g(2)$/100 g sln and the corresponding mole fraction, x_2, is $3.3 \cdot 10^{-4}$ (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The Karl Fischer dead-stop back-titration method was used. 50 mL of (1) was placed in the equilibration vessel. A test tube containing 6 mL of (2) was then placed in the vessel so that the rim of the tube rested against the upper inside wall of the vessel. The vessel was then stoppered, placed inside a plastic bag and submerged in a water thermostat. Trials had shown that the concentration of (2) in (1) became constant within 2 days. 10 mL of (1) saturated with (2) were transferred to the titration vessel for water determination. Apparatus is described in the paper.

Source and Purity of Materials:

(1) Fisher C-555; purified by double crystallization; purity 99.6% (gas chromatographic analysis); d_4^{25} 0.7734± 0.00001.
(2) Distilled and de-ionized.

Estimated Error:

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

References:

[1]S. Goldman, Can. J. Chem. **52**, 1668 (1974).

Components:	Original Measurements:
(1) Cyclohexane; C_6H_{12} ; [110-82-7] (2) Water; H_2O; [7732-18-5]	I. M. Korenman and R. P. Aref'eva, Patent USSR, 553 524, 5 April 1977.
Variables:	**Prepared By:**
One temperature: 20 °C	A. Maczynski

Experimental Data

The solubility of cyclohexane in water at 20 °C was reported to be 0.10 $g(1)$/mL(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.010 $g(1)$/100 g sln and $2.1 \cdot 10^{-5}$. The compiler's calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

About 100–500 mL (2) was placed in a glass cylinder and 10–50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2–3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5–1.5 min.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Cyclohexane; C_6H_{12} ; [110-82-7] (2) Water; H_2O; [7732-18-5]	I. M. Korenman and R. P. Aref'eva, Zh. Prikl. Khim. (Leningrad) **51**, 957 (1978).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of cyclohexane in water at 25 °C was reported to be 0.12 $g(1)$/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.012 $g(1)$/100 g sln and $2.6 \cdot 10^{-5}$. The compilers' calculations assume a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

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

Components:	**Original Measurements:**
(1) Cyclohexane; C_6H_{12} ; [110-82-7] (2) Water; H_2O; [7732-18-5]	A. P. Kudchadker and J. J. McKetta, AIChE J. **7**, 707 (1961).
Variables:	**Prepared By:**
Temperature: 310.93 °C–410.93 °C Pressure: 14.7 psia–450 psia	M. C. Haulait-Pirson

Experimental Data

Solubility of cyclohexane in water. Smoothed data.

T/K	$10^5 \cdot x_1$	$g(1)$/100 g sln (compiler)	P/psia	P/MPa (compiler)
310.93	0.97	0.00454	14.7	0.101
	1.34	0.00626	20.0	0.138
	2.03	0.00949	30.0	0.207
	2.72	0.01272	40.0	0.276
	3.41	0.01594	50.0	0.345
	4.10	0.01917	60.0	0.414
	5.48	0.02562	80.0	0.552
	6.85	0.03202	100.0	0.689
	8.22	0.03842	120.0	0.827
	9.60	0.04487	140.0	0.965
	11.03	0.05155	160.0	1.103
	12.04	0.05627	180.0	1.241
	13.8	0.06449	200.0	1.379
	17.08	0.07981	250.0	1.724
	20.2	0.09438	300.0	2.068
	23.11	0.10796	350.0	2.413
	25.84	0.12070	400.0	2.758
	28.35	0.13241	450.0	3.103
344.26	0.58	0.00271	14.7	0.101
	1.00	0.00468	20.0	0.138
	1.60	0.00748	30.0	0.207
	2.20	0.01029	40.0	0.276
	2.93	0.01323	50.0	0.345
	3.45	0.01613	60.0	0.414
	4.71	0.02202	80.0	0.552
	5.92	0.02767	100.0	0.689
	7.18	0.03356	120.0	0.827
	8.43	0.03940	140.0	0.965
	9.71	0.04538	160.0	1.103
	10.92	0.05104	180.0	1.241
	12.28	0.05739	200.0	1.379
	15.41	0.07201	250.0	1.724
	18.24	0.08522	300.0	2.068
	21.0	0.09811	350.0	2.413
	23.61	0.11029	400.0	2.758
	25.98	0.12135	450.0	3.103
377.59			14.7	0.101
	—	—	20.0	0.138
	0.72	0.00337	30.0	0.207
	1.32	0.00617	40.0	0.276
	1.92	0.00898	50.0	0.345
	2.51	0.01173	60.0	0.414

	3.70	0.01730	80.0	0.552
	4.89	0.02286	100.0	0.689
	6.05	0.02828	120.0	0.827
	7.27	0.03398	140.0	0.965
	8.48	0.03964	160.0	1.103
	9.69	0.04529	180.0	1.241
	10.8	0.05048	200.0	1.379
	13.92	0.06505	250.0	1.724
	16.68	0.07794	300.0	2.068
	19.2	0.08971	350.0	2.413
	21.52	0.10054	400.0	2.758
	23.46	0.10959	450.0	3.103
410.93	0.70	0.00327	60.0	0.414
	1.91	0.00893	80.0	0.552
	3.13	0.01463	100.0	0.689
	4.40	0.02057	120.0	0.827
	5.62	0.02627	140.0	0.965
	6.82	0.03188	160.0	1.103
	7.95	0.03716	180.0	1.241
	9.08	0.04244	200.0	1.379
	12.1	0.05655	250.0	1.724
	14.6	0.06823	300.0	2.068

Auxiliary Information

Method/Apparatus/Procedure:

The experimental technique and the analytical procedure are described in detail in Davis.[1] No more details are given in the paper.

Source and Purity of Materials:

(1) Pure grade stock; purity of about 99.6% (gas chromatography).
(2) Distilled; boiled to remove any dissolved gases.

Estimated Error:

Not specified.

References:

[1]J. E. Davis, M. S. Thesis, The University of Texas, Austin, 1959.

Components:

(1) Cyclohexane; C_6H_{12}; [110-82-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

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

Variables:

One temperature: 25 °C

Prepared By:

M. C. Haulait-Pirson

Experimental Data

The solubility of cyclohexane in water at 25 °C was reported to be 56.7 mg(1)/L sln.

With the assumption of a solution density of 1.00 g/mL, the corresponding mass percent is 0.00567 $g(1)$/100 g sln and the corresponding mole fraction, x_1, is $1.21 \cdot 10^{-5}$ (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was equilibrated for at least 12 h in a 200 mL Teflon stoppered vessel with gentle shaking. The solution was allowed to settle for 6 h and the aqueous phase was tested (Tyndall effect). Both phases were analyzed by the gas chromatographic technique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analyzed by glc. The instrument was a Hewlett-Packard model equipped with a flame ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; research grade; purity 99+%; used without further purification.
(2) Doubly distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: ±1 mg(1)/L sln.

Components:	Original Measurements:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	D. Mackay and W. Y. Shiu, Can. J. Chem. Eng. **53**, 239 (1975).
Variables:	**Prepared By:**
One temperature: 25 °C	M. C. Haulait-Pirson

Experimental Data

The solubility of cyclohexane in water at 25 °C was reported to be 0.0575 $g(1)$/L sln.

With the assumption of a solution density of 1.00 g/mL, the corresponding mass percent is 0.00575 $g(1)$/100 g sln and the corresponding mole fraction, x_1, is $1.23 \cdot 10^{-5}$ (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of (1) in (2) was determined using a vapor phase extraction technique followed by gas chromatographic analysis. Equilibration apparatus and procedure are given in detail in the paper. The gas chromatograph was a Hewlett-Packard instrument equipped with a hydrogen flame-ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; research grade >99.9%; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 0.0073 $g(1)$/L sln.

Components:	Original Measurements:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	D. Mackay, W. J. Shiu, and A. W. Wolkoff, ASTM Spec. Tech. Pub. **573**, 251 (1975).
Variables:	**Prepared By:**
Not specified	M. C. Haulait-Pirson

Experimental Data

The authors reported three different values for the solubility of cyclohexane in water: 55.8, 50.2, and 61.7 mg(1)/L sln.

Using the mean value and assuming a solution density of 1.00 g/mL, the corresponding mass percent, calculated by the compiler, is 0.0056 $g(1)$/100 g sln and the corresponding mole fraction, x_1, is $1.2 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

(1) was partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equilibrations it was possible to calculate the amount of (1) in the original sample.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Solubility: ±10% (compiler).

Components:
(1) Cyclohexane; C_6H_{12}; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of cyclohexane in water at 25 °C was reported to be 55 mg(1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is $1.18 \cdot 10^{-5}$.

The same value is also reported in McAuliffe.[1,2]

Auxiliary Information

Method/Apparatus/Procedure:
In a 250 mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton syringe and injected into a gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

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

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 2.3 mg(1)/kg sln (standard deviation of mean).

References:
[1]C. McAuliffe, Nature (London) **200**, 1092 (1963).
[2]C. McAuliffe, Am. Chem. Soc. Div. Petrol. Chem. **9**, 275 (1964).

Components:
(1) Cyclohexane; C_6H_{12}; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of cyclohexane in water at 25 °C was reported to be 0.008 $g(1)$/100 ml sln.

With the assumption of a solution density of 1.00 g/mL, the corresponding mass percent is 0.008 $g(1)$/100 g sln and the corresponding mole fraction, x_1, is $1.7 \cdot 10^{-5}$ (compiler).

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 278.26 K–318.36 K

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of cyclohexane in water

T/K	$10^3 \cdot x_1$	$g(1)$/100 g sln
278.26	0.01837	0.008193 ± 0.00017
288.36	0.01991	0.008870 ± 0.00025
298.26	0.01998	0.008884 ± 0.00024
308.36	0.02004	0.008884 ± 0.00025
318.36	0.02068	0.009132 ± 0.00025

Auxiliary Information

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

Source and Purity of Materials:
(1) Fisher Scientific Co.; certified grade; used as received.
(2) Laboratory distilled water.

Estimated Error:
Solubility: standard deviations from at least 15 measurements are given above.

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. M. Plenkina, R. O. Pryanikova, and G. D. Efremova, Zh. Fiz. Khim. **45**, 2389 (1971); Deposited doc. 1971, VINITI 3028-71.

Variables:
Temperature: 130 °C–250 °C

Prepared By:
A. Maczynski

Experimental Data

Solubility of water in cyclohexane

t/°C	x_2	$g(2)$/100 g sln (compiler)
130	0.036	0.79
163.0	0.093	2.15
188.0	0.130	3.10
200.9	0.154	3.75
213.5	0.193	4.87
219.0	0.216	5.52
232.0	0.265	7.16
244.0	0.322	9.23
250.0	0.350	10.33

Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; CP reagent; crystallized several times; m.p. 6.50 °C.
(2) Distilled.

Estimated Error:
Temperature: ±0.5 °C.

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. J. Rebert and K. E. Hayworth, AIChE J. **13**, 118 (1967).

Variables:
Pressure and temperature on one phase-two phase boundary

Prepared By:
C. L. Young

Experimental Data

Smoothed data

t/°C	T/K	x_1	$g(1)$/100 g sln	P/MPa
320	593	0.0059	2.7	11.43
330	603	0.0059	2.7	13.06
340	613	0.0059	2.7	14.92
350	623	0.0059	2.7	16.86
360	633	0.0059	2.7	19.21
370	643	0.0059	2.7	21.83
370.6	643.8[a]	0.0059	2.7	22.14
320	643	0.0059	2.7	22.06
360	633	0.0059	2.7	20.07
350	623	0.0059	2.7	18.25
340	613	0.0059	2.7	16.65
330	603	0.0059	2.7	15.23
320	593	0.0059	2.7	14.17
310	583	0.0059	2.7	13.39
307	580	0.0059	2.7	13.24
304	577	0.0059	2.7	13.21
302	575	0.0059	2.7	13.28
300	573	0.0059	2.7	13.69
295	568	0.0059	2.7	15.88
292	565	0.0059	2.7	17.52
290	563	0.0059	2.7	18.63
330	603	0.0059	2.7	13.46
340	613	0.021	9.0	15.44
350	623	0.021	9.0	17.70
360	633	0.021	9.0	20.61
362	635	0.021	9.0	21.38
363.3	636.5	0.021	9.0	21.94
362	635	0.021	9.0	22.32
360	633	0.021	9.0	22.45
359.4	632.6[a]	0.021	9.0	22.49
359	632	0.021	9.0	22.51
358	631	0.021	9.0	22.54
356	629	0.021	9.0	22.62
354	627	0.021	9.0	22.71
352	625	0.021	9.0	22.81
350	623	0.021	9.0	22.96
348	621	0.021	9.0	23.16
346	619	0.021	9.0	23.48
235	507	0.0966	33.3	3.68
245	517	0.0966	33.3	4.36
255	527	0.0966	33.3	5.18
265	537	0.0966	33.3	6.10
275	547	0.0966	33.3	7.12
285	557	0.0966	33.3	8.25

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of cyclohexane in water at 25 °C and at system pressure was reported to be 66.5 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.00665 $g(1)$/100 g sln and $1.423 \cdot 10^{-5}$.

Auxiliary Information

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

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

Estimated Error:
Temperature: ±1 °C.
Solubility: ±0.8 mg(1)/kg(2).

295	567	0.0966	33.3	9.57
300	573	0.0966	33.3	10.30
305	578	0.0966	33.3	11.07
310	583	0.0966	33.3	11.96
315	588	0.0966	33.3	12.87
320	593	0.0966	33.3	13.79
325	598	0.0966	33.3	14.96
330	603	0.0966	33.3	16.13
335	608	0.0966	33.3	17.50
340	613	0.0966	33.3	19.07
220	493	0.0243	60.0	3.68
230	503	0.0243	60.0	4.47
240	513	0.0243	60.0	5.35
250	523	0.0243	60.0	6.30
260	533	0.0796	94.8	7.45
270	543	0.0796	94.8	8.78
280	553	0.0796	94.8	10.29
290	563	0.0796	94.8	12.17
300	573	0.0796	94.8	14.32
310	583	0.0796	94.8	17.79
220	493	0.0796	94.8	2.42
230	503	0.0796	94.8	2.88
240	513	0.0796	94.8	3.42
250	523	0.0796	94.8	4.09
260	533	0.0796	94.8	4.86
262	535	0.0796	94.8	5.06
264	537	0.0796	94.8	5.28
266	539	0.0796	94.8	5.54
268.9	542.1	0.0796	94.8	6.25
268	541	0.0796	94.8	6.60
267.2	540.4	0.0796	94.8	6.73
267	540	0.0796	94.8	6.76
263	536	0.0796	94.8	7.06
261	534	0.0796	94.8	7.08
260	533	0.0796	94.8	7.06
255	528	0.0796	94.8	6.93
250	523	0.0796	94.8	6.76
245	518	0.0796	94.8	6.56
243.2	516.4[b]	0.0796	94.8	6.48

Three phase equilibrium locus

t/°C	T/K	P/MPa
130	403	0.66
140	413	0.86
150	423	1.08
160	433	1.32
170	443	1.63
180	453	2.01
190	463	2.46
200	473	2.99
210	483	3.58
220	493	4.32
230	503	5.18
235	508	5.64
240	513	6.14
245	518	6.68
250	523	7.28
255	528	7.92
255.7	528.9	8.01

[a]Critical point.

[b]Three-phase point.

Auxiliary Information

Method/Apparatus/Procedure:

Samples of mixtures of known composition were confined over mercury. Samples were heated in a vapor bath and the pressure–temperature phase boundaries determined by direct observation of appearance or disappearance of a phase. Apparatus similar to that described in Rebert and Kay.[1]

Source and Purity of Materials:

(1) No details given.

Estimated Error:

Temperature: δT/K= ± 0.05.
Pressure: δP/psi= ± 1.

References:

[1]C. J. Rebert and W. B. Kay, AIChE J. **5**, 285 (1959).

Components:
(1) Cyclohexane; C_6H_{12}; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of water in cyclohexane at 25 °C was reported to be 0.00345 mol(2)/L sln corresponding to a mole fraction, x_2, of $3.75 \cdot 10^{-4}$.

The corresponding mass percent value calculated by the compiler is 0.0080 $g(2)$/100 g sln.

The compiler's calculation assumes a solution density of 0.7739 g/mL. (density of cyclohexane reported in Goldman[1]).

Auxiliary Information

Method/Apparatus/Procedure:
A method of gravimetric absorption monitored by tritium tracer was used. (1) was equilibrated with a slight excess of titrated water by shaking over a period of at least 8 h in a thermostat. The phases were allowed to separate for at least 16 h and then were sampled for tritium analysis. Most of the (1) phase was weighed into a boiling flask of a closed distillation system and then distilled through a magnesium perchlorate weighing tube. The magnesium perchlorate was then dissolved for measurement of its tritium content by liquid scintillation counting with a Packard Tri-Carb Scintillation Spectrometer.

Source and Purity of Materials:
(1) Source not specified; spectral grade reagent.
(2) Tritiated water at 5 Ci/mL; New England Nuclear Corp.; diluted to about 1 mCi/L.

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

References:
[1]S. Goldman, Can. J. Chem. **52**, 1968 (1974).

Components:
(1) Cyclohexane; C_6H_{12}; [110-82-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The authors reported the partition coefficient α of cyclohexane between the gas and aqueous phase. $\alpha = 8.0 \pm 02$. $\alpha = C_g/C_s$, with C_s being the concentration of the compound in dilute aqueous solution at 25 °C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of P (where P is the vapor pressure in mm of Hg) is taken from Ref. 1. $P = 97.58$ mm of Hg and $\log C_g = \log P - 4.269 = -2.28$ expressed in moles per liter. Therefore $C_s = 6.56 \cdot 10^{-4}$ moles/L. With the assumption of a solution density of 1.00 g/$\cdot$ mL, the corresponding mass percent is 0.0055 $g(1)$/100 g sln and the corresponding mole fraction, x_1, is $1.2 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
The equilibrium distribution was attained after shaking for 10 min a thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.

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

Estimated Error:
Solubility: ± 10% (estimated by the compiler).

References:
[1]J. Hine and P. K. Mooker, J. Org. Chem. **4**, 292 (1975).

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of cyclohexane in water

t/°C	mol(1)/L sln	$g(1)/100$ g sln (compilers)	x_1 (compilers)
25.0	$6.27 \cdot 10^{-4}$	$5.29 \cdot 10^{-3}$	$1.133 \cdot 10^{-5}$

Auxiliary Information

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

Source and Purity of Materials:
(1) Source not specified; analytical reagent grade; purity 98%; used as received.
(2) Deionized and redistilled.

Estimated Error:
Temperature: ±0.1 °C.

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

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 23.5 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of cyclohexane in water at 23.5 °C was reported to be 0.0052±0.0002 $g(1)/100$ g sln.
The corresponding mole fraction, x_1 was calculated by the compiler to be $1.1 \cdot 10^{-5}$.

Auxiliary Information

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

Source and Purity of Materials:
(1) 99.9% purity used without further purification.
(2) Distilled.

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

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 200°C–250 °C
Pressure: 2.8 MPa–78.5 MPa

Prepared By:
A. Maczynski

Experimental Data
Solubility of water in cyclohexane

t/°C	x_2	$g(2)$/100 g sln (compiler)	P/kg^{-2}	P/MPa (compiler)
200	0.156	3.81	29	2.8
200	0.091	2.10	50	4.9
200	0.052	1.16	100	9.8
200	0.046	1.02	150	14.7
200	0.043	0.95	200	19.6
200	0.042	0.93	300	29.4
200	0.042	0.93	400	39.2
200	0.042	0.93	500	49.0
200	0.042	0.93	600	58.8
200	0.042	0.93	700	68.6
200	0.041	0.91	800	78.5
225	0.230	6.01	46.2	4.5
225	0.209	5.35	50	4.9
225	0.128	3.05	100	9.8
225	0.100	2.32	150	14.7
225	0.087	2.00	200	19.6
225	0.084	1.92	300	29.4
225	0.080	1.83	400	39.2
225	0.076	1.73	500	49.0
225	0.072	1.63	600	58.8
225	0.068	1.54	700	68.6
225	0.055	1.23	800	78.5
250	0.345	10.13	70	6.9
250	0.232	6.07	100	9.8
250	0.182	4.55	150	14.7
250	0.165	4.06	200	19.6
250	0.145	3.50	300	29.4
250	0.131	3.13	400	39.2
250	0.122	2.89	500	49.0
250	0.114	2.68	600	58.8
250	0.106	2.47	700	68.6
250	0.100	2.32	800	78.5

Auxiliary Information

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

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

Estimated Error:
Not specified.

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

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 40.0 °C

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

Experimental Data
Solubility of water in cyclohexane

t/°C	$g(2)$/100 g sln	x_2 (compilers)
40.0	$6\cdot10^{-5}$	$2.8\cdot10^{-4}$

Auxiliary Information

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

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

Estimated Error:
Temperature: ±0.1 °C.

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

Components
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 14 °C–53 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of water in cyclohexane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
14	2.3	0.005
19	4.7	0.010
28.5	7.0	0.015
32.5	9.3	0.020
38	14.5	0.031
53	23.3	0.050

Auxiliary Information

Method/Apparatus/Procedure:
No details were reported in the paper.

Source and Purity of Materials:
(1) Kahlbaum; dried over calcium chloride and twice distilled over Na–K.
(2) Not specified.

Estimated Error:
Solubility: ±0.01%.

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 313 K–482 K
Pressure: 0.03 MPa–3.0 MPa

Prepared By:
G. T. Hefter

Experimental Data

The solubility of cyclohexane in water

T/K	$10^4 \cdot x_1$	$10^2 \cdot$ g(1)/100 g sln (compiler)	P/MPa
313.15	0.156[b]	0.728	0.03151
373.15	0.379[b]	1.77	0.2723
422.04	1.03	4.81	—[a]
423.15	1.30	6.07	1.0032
473.15	3.92	18.3	2.965
482.21	4.93	23.0	—[a]

[a]Not specified.
[b]Other data presented but rejected by the authors.

The solubility of water in cyclohexane

T/K	$10^3 \cdot x_2$	$g(2)$/100 g sln (compiler)	P^a/MPa
313.15	0.887	0.021[a]	0.03151
	0.924		
	1.13		
373.15	4.35	0.10[a]	0.2723
	5.12		
423.15	20.4	0.47[a]	1.0082
	24.0		
473.15	79.3	1.81	2.965

[a]Average value.

The three phase critical point was reported to be 529.4 K, 8.025 MPa, and $x_1 = 1.748 \cdot 10^{-3}$ (0.82 $g(1)$/100 g sln, compiler).
The authors also report an equation fitted to their own and literature data over the range 273–529 K, vis.

$$\ln x_1 = -209.11689 + 8325.49/T + 29.8231 \ln T$$

$$\ln x_2 = -62.7645 - 654.027/T + 9.99967 \ln T$$

Auxiliary Information

Method/Apparatus/Procedure:
All experimental details are given in an Appendix deposited in a Documentation Center rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, while that of (2) in (1) was measured by the Karl Fischer method.

Source and Purity of Materials:
(1) No details given.
(2) No details given.

Estimated Error:
Temperature: not stated.
Solubility: ±5% relative; repeatability of replicate analyses.
Pressure: ±1%; type of error not stated.

Components:
(1) Cyclohexane; C_6H_{12}; [110-82-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Ya. D. Zel'venskii, A. A. Efremov, and G. M. Larin, Khim. Tekhnol. Topl. Masel **10**, 3 (1965).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Data

The solubility of water in cyclohexane at 20 °C was reported to be 0.0098 $g(2)$/100 g sln.

The corresponding mole fraction, x_2 calculated by the compiler is $4.6 \cdot 10^{-4}$.

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions of tritum labeled (2) in (1) were prepared in two ways. In the first, nitrogen was passed through the vessel with (2) and next through the vessel with (1) and frozen. In the second, about 500 mL of (1) and 1 μL (2) were stirred. The concentration of (2) in (1) was calculated from scintillation measurements.

Source and Purity of Materials:

(1) Source not specified; pure grade; shaken with concentration $H_2SO_4 + HNO_3$; washed with water, dried over sodium, and distilled; purity not specified. Boiling point 80.82 °C.
(2) Source not specified; commercial; 1 C_i/mL HTO; used as received.

Estimated Error:
Not specified.

Components:
(1) Cyclohexane; C_6H_{12}; [110-82-7]
(2) Heavy water (deuterium oxide); D_2O; [7789-20-0]

Original Measurements:
P. Backx and S. Goldman, J. Phys. Chem. **85**, 2975 (1981).

Variables:
Temperature: 283 K–313 K

Prepared By:
A. Maczynski

Experimental Data

Solubility of heavy water in cyclohexane

T/K	$10^4 \cdot x_2$	Standard dev	$10^4 \cdot g(2)$/100 g sln (compiler)
283	1.57	0.08	0.374
288	1.81	0.10	0.431
293	2.42	0.10	0.576
298	2.80	0.11	0.666
303	3.61	0.24	0.859
308	4.64	0.56	1.104
313	5.35	0.24	1.274

Auxiliary Information

Method/Apparatus/Procedure:

In a 175 mL milk-dilution bottle fitted with a Bakelite screw cap and a Teflon insert and rotated end-over-end, (1) was equilibrated with an excess of (2), sampled with Hamilton syringes and titrated in an Aquatest II automatic Karl Fischer Titrator.

Source and Purity of Materials:

(1) Certified grade; washed with water, dried with silica gel, and distilled; d^{25} 0.77390.
(2) Obtained from the manufacturer; minimum isotopic purity of 99.7 atom % D.

Estimated Error:

Temperature: ±0.01 K.
Solubility: standard deviation calculated from 18 to 32 determinations reported above.

Components:
(1) Cyclohexane; C_6H_{12} ; [110-82-7]
(2) Heavy water (deuterium oxide); D_2O; [7789-20-0]

Original Measurements:
A. N. Guseva and E. I. Parnov, Radiokhimiya **5**, 507 (1963).

Variables:
Temperature: 71 °C–179.5 °C

Prepared By:
A. Maczynski

Experimental Data

Solubility of cyclohexane in heavy water

t/°C	$10^4 \cdot x_1$	$g(1)$/100 g sln (compiler)
71	0.331	0.0139
143	1.48	0.0622
168	3.2	0.134
179.5	4.47	0.188

Auxiliary Information

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

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

Estimated Error:
Not specified.

3.6. 2,3-Dimethyl-1-butene

Components:
(1) 2,3-Dimethyl-1-butene; C_6H_{12} ; [563-78-0]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 30 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in 2,3-dimethyl-1-butene at 30 °C was reported to be 0.0459 $g(2)$/100 g sln.
The corresponding whole fraction, x_2 calculated by the compilers is $2.14 \cdot 10^{-3}$.

Auxiliary Information

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

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

Estimated Error:
Not specified.

3.7. 1-Hexene*

Components:	**Evaluators:**
(1) 1-Hexene; C_6H_{12} ; [592-41-6]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, July, 2003.
(2) Water; H_2O; [7732-18-5]	

Critical Evaluation of the Solubility of 1-Hexene (1) in Water (2)

Listed below are the experimental solubility data for (1) in (2) which have been investigated by the authors, together with temperature range and pressure range, if reported:

Author (s)	T/K	Author (s)	T/K
Budantseva *et al.*[1]	298	McAuliffe[5]	278–318
Economou *et al.*[2]	311–496 (207–5378 kPa)	Natarajan and Venkatachalam[6]	298–426
Leinonen and Mackay[4]	298	Tewari *et al.*[7]	298

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

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

where: $\ln x_{1,\min} = -11.41$; $\Delta_{sln} C_P / R = 43.4$; $T_{\min} = 306$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference data are listed in Table 11. All the data are shown in Fig. 5. The data of Leinonen and Mackay,[4] McAuliffe[5] and Natarajan and Venkatachalam[6] at 298 K are in good agreement with each other and with the reference data (within 30% relative standard deviation) and are Recommended. The data of of Budantseva *et al.*[1] and Economou[2] are in good agreement with the reference data and are Tentative. The data of Tewari *et al.*[7] at 298 K are in poor agreement with the reference data and are Doubtful.

Critical Evaluation of the Solubility of Water (2) in 1-Hexene (1)

The experimental solubility for (1) in (2) have been investigated by Budantseva *et al.*[1] at 293 K, Englin *et al.*[3] at 303 K, and Economou *et al.*[2] at 311 K–496 K and 207 kPa–5378 kPa.

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

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

where: $d_1 = -1.118$; $d_2 = -3.190$; $d_3 = 0.602$; $d_4 = -9.144$; $T_r = T/497.1$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of 1-hexene in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 12. All the data are shown in Fig. 6. The data of Budantseva *et al.*,[1] Economou *et al.*[2] at 367 and 420 K, and Englin *et al.*[3] are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Economou *et al.*[2] at 311 K, 475 K, and 496 K are in poor agreement with the reference data and are Doubtful.

TABLE 11. Experimental values for solubility of 1-hexene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
293.2		$1.00 \cdot 10^{-5}$ (T; Ref. 1)	$1.2 \cdot 10^{-5}$
298.2		$1.18 \cdot 10^{-5}$ (R; Ref. 4), $9.20 \cdot 10^{-6}$ (R; Ref. 5), $1.40 \cdot 10^{-5}$ (R; Ref. 6), $1.50 \cdot 10^{-5}$ (D; Ref. 7)	$1.1 \cdot 10^{-5}$
310.9	206.8 (Ref. 2)	$1.20 \cdot 10^{-5}$ (T; Ref.2)	$1.1 \cdot 10^{-5}$
366.5		$2.40 \cdot 10^{-5}$ (T; Ref.2)	$2.2 \cdot 10^{-5}$
422.0		$8.50 \cdot 10^{-5}$ (T; Ref.2)	$8.4 \cdot 10^{-5}$
477.6		$4.40 \cdot 10^{-4}$ (T; Ref.2)	$4.6 \cdot 10^{-4}$
494.3		$7.30 \cdot 10^{-4}$ (T; Ref.2)	$8.0 \cdot 10^{-4}$

References:

[1]L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).
[2]I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).
[3]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[4]P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. **51**, 230 (1973).
[5]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[6]G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).
[7]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

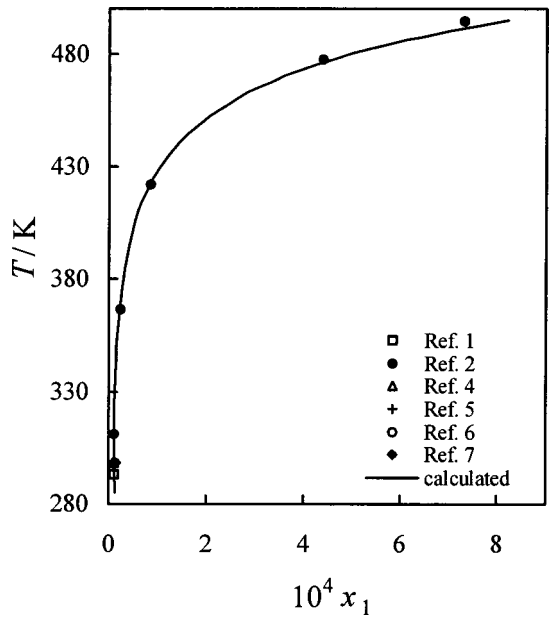

FIG. 5. All the solubility data for 1-hexene (1) in water (2).

TABLE 12. Experimental values for solubility of water (2) in 1-hexene (1)

T/K	P/kPa	Experimental values x_2 (T = tentative, D = doubtful)	Reference values $x_2 \pm 30\%$
293.2		$1.60 \cdot 10^{-3}$ (T; Ref. 1)	$1.3 \cdot 10^{-3}$
303.2		$2.23 \cdot 10^{-3}$ (T; Ref. 3)	$1.9 \cdot 10^{-3}$
310.9	206.8 (Ref. 2)	$1.437 \cdot 10^{-3}$ (D; Ref. 2)	$2.4 \cdot 10^{-3}$
366.7	318.4 (Ref. 2)	$1.015 \cdot 10^{-2}$ (T; Ref. 2)	$1.4 \cdot 10^{-2}$
420.4	1247.3 (Ref. 2)	$4.329 \cdot 10^{-2}$ (T; Ref. 2)	$6.2 \cdot 10^{-2}$
475.3	3923 (Ref. 2)	$1.533 \cdot 10^{-1}$ (D; Ref. 2)	$2.3 \cdot 10^{-1}$
496.3	5378 (Ref. 2)	$2.207 \cdot 10^{-1}$ (D; Ref. 2)	$3.4 \cdot 10^{-1}$

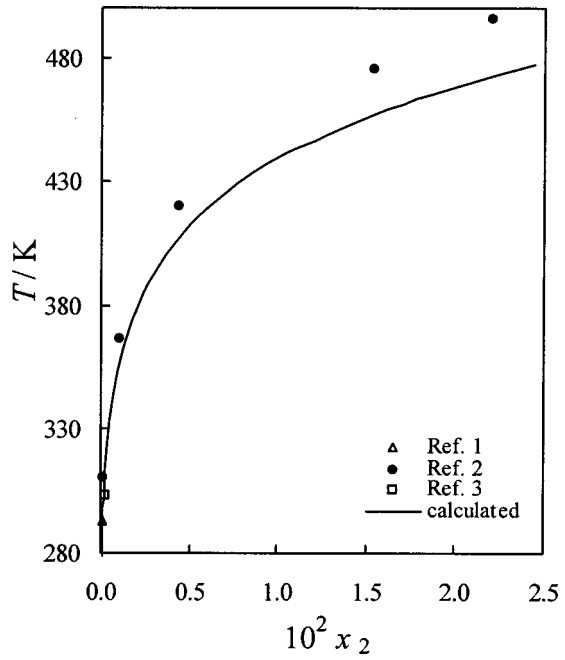

FIG. 6. All the solubility data for water (2) in 1-hexane (1).

Components:
(1) 1-Hexene; C_6H_{12}; [592-41-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. S. Budantseva, T. M. Lesteva, and M. S. Nemtsov, Zh. Fiz. Khim. **50**, 1344 (1976).

Variables:
One temperature: 20 °C

Prepared By:
A. Maczynski

Experimental Data

The solubility of 1-hexene in water at 20 °C was reported to be $x_1 = 1 \cdot 10^{-5}$.

The corresponding mass percent calculated by the compiler is 0.005 $g(1)$/100 g sln.

The solubility of water in 1-hexene at 20 °C was reported to be $x_2 = 0.0016$.

The corresponding mass percent calculated by the compiler is 0.029 $g(2)$/100 g sln.

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components:
(1) 1-Hexene; C_6H_{12}; [592-41-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. G. Economou, J. L. Heidman, C. Tsonopoulos, and G. M. Wilson, AIChE J. **43**, 535 (1997).

Variables:
Temperature: 310.93 K–496.26 K
Pressure: 0.2068 MPa–5.378 MPa

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

Experimental Data

Solubility of 1-hexene in water

T/K	P/MPa	$g(1)$/100 g sln (compilers)	$10^4 \cdot x_1$
310.93	0.2068	0.0056	0.12
366.48	—	0.0112	0.24
422.04	—	0.0397	0.85
477.59	—	0.205	4.4
494.26[a]	—	0.340	7.3

Solubility of water in 1-hexene

T/K	P/MPa	$g(2)$/100 g sln (compilers)	x_2
310.93	0.2068	0.03079	0.001437
366.65	0.3184	0.2192	0.01016
420.37	1.2473	0.9593	0.04329
475.26	3.923	3.731	0.1533
496.26[a]	5.378	5.716	0.2207
493.32[b]	5.316	8.85	0.312

[a]Above three-phase critical end point.

[b]Measured three-phase critical end point.

Auxiliary Information

Method/Apparatus/Procedure:
The experimental procedure was described in Tsonopoulos and Wilson[1] and Heidman *et al.*[2] The solubility of hydrocarbon in water was measured by glc, while that of water in hydrocarbon by the Karl Fischer titration. The three-phase critical end points were determined in the visual cell apparatus. Data other than three-phase critical end point were previously reported in Brady *et al.*[3]

Source and Purity of Materials:
(1) Aldrich; purity >99 mole % by glc.
(2) Distilled.

Estimated Error:
Temperature: ±0.6 K at critical end point.[b]
Solubility: 5% (repeatability) and ±0.02 mole fraction at critical end point.[b]
Pressure: 1% and ±0.04 MPa at critical end point.[b]

References:
[1]C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).
[2]J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).
[3]C. J. Brady, J. R. Cunningham, and G. M. Wilson, GPA/API Res. Proj. RR-62, Gas Processors Assoc., Tulsa, OK (1982).

Components:
(1) 1-Hexene; C_6H_{12}; [592-41-6]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 30 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in 1-hexene at 30 °C was reported to be 0.0477 $g(2)$/100 g sln.
The corresponding mole fraction, x_2, calculated by the compilers is $2.23 \cdot 10^{-3}$.

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components:	Original Measurements:
(1) 1-Hexene; C_6H_{12}; [592-41-6] (2) Water; H_2O; [7732-18-5]	P. J. Leinonen and D. Mackay, Can. J. Chem. Eng. **51**, 230 (1973).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of 1-hexene in water at 25 °C was reported to be 55.4 mg(1)/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00554 $g(1)$/100 g sln and $1.18 \cdot 10^{-5}$. The compiler's calculation assumes a solution density of 1.00 g/mL.

Auxiliary Information

Method/Apparatus/Procedure:

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

Source and Purity of Materials:

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

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 30 mg(1)/L sln (2 standard deviations).

Components:	Original Measurements:
(1) 1-Hexene; C_6H_{12}; [592-41-6] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of 1-hexene in water at 25 °C was reported to be 50 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0050 $g(1)$/100 g sln and $9.2 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 1.2 mg(1)/kg(2) (standard deviation of mean).

Components:
(1) 1-Hexene; C_6H_{12}; [592-41-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).

Variables:
One temperature: 25 °C

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

Experimental Data

The solubility of 1-hexene in water was reported to be $7.781 \cdot 10^{-4}$ mol/L at 25 °C. (It should be noted that although the authors state that the solubility refers to "water" the context in the paper is ambiguous and the data were probably obtained in 0.001 mol·/L HNO_3 solution.)

Assuming a solution density of 1.00 g/mL the corresponding mass percent and mole fraction (x_1) solubilities calculated by the compilers are, respectively, 0.00654 $g(1)$/100 g sln and $1.40 \cdot 10^{-5}$.

Solubility data are also presented as a function of temperature in various salt solutions.

Auxiliary Information

Method/Apparatus/Procedure:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the (1) content determined by titration with bromine using standard procedures.

Source and Purity of Materials:
(1) Matheson, Coleman, and Bell; 99%.
(2) Not specified.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: not specified.

Components:
(1) 1-Hexene; C_6H_{12}; [592-41-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:
One temperature: 25.0 °C

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

Experimental Data

Solubility of 1-hexene in water

t/°C	mol(1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$8.28 \cdot 10^{-4}$	$6.99 \cdot 10^{-3}$	$1.496 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
A generator column method was used as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with (1) by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by glc. The column was thermostated by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

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

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:
[1]H. De Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

3.8. 2-Hexene

Components:
(1) 2-Hexene; C_6H_{12}; [592-43-8]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
G. S. Natarajan and K. A. Venkatachalam, J. Chem. Eng. Data **17**, 328 (1972).

Variables:
Temperature: 20 °C–30 °C

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

Experimental Data

Solubility of 2-hexene in 0.001 mol/L HNO_3 solution.

t/°C	$10^5 \cdot x_1$ (compiler)	$10^3 \cdot g(1)/100$ g sln[b] (compiler)	$10^4 \cdot$ mol(1)/L sln[a]
20	1.6	7.4	8.75±0.21
25	1.4	6.7	7.99±0.23
30	1.2	5.5	6.60±0.26

[a]Uncertainties stated to be "standard deviations from means."
[b]Assuming a solution density of 1.00 g/mL at all temperatures.

Compiler's note: Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause the solubility of (1) to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol/L HCl.

Auxiliary Information

Method/Apparatus/Procedure:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the (1) content determined by titration with bromine using standard procedures.

Source and Purity of Materials:
(1) Prepared by dehydration of 2-hexanol and then washed, dried, and fractionated. Purity (no specification) was determined by chromatography.
(2) Not specified.

Estimated Error:
Temperature: ±0.05 °C.
Solubility: see table above.

3.9. Methylcyclopentane*

Components:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7]
(2) Water; H_2O; [7732-18-5]

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

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

Listed below are the experimental solubility data for (1) in (2) which have been investigated by the authors.

Author (s)	T/K	Author (s)	T/K
Guseva and Parnov[2]	335–472	Price[4]	298
McAuliffe[3]	298	Rudakov and Lutsyk[5]	298

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

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

where: $\ln x_{\min,1} = -11.56$; $\Delta_{sln}C_P/R = 38.1$; $T_{\min} = 298$ K.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the reference data. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

All the data are in Table 13 and shown in Fig. 7. The data of McAuliffe,[3] Price,[4] and Rudakov and Lutsyk[5] and are in good agreement with each other and with the reference data (within 30% relative standard deviation) and are Recommended. The data of Guseva and Parnov[2] are in poor agreement with the reference data and are Doubtful.

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

The experimental solubility for (2) in (1) has been investigated by Englin *et al.*[1] at 283 K–303 K.

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

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

where: $d_1 = -1.054$; $d_2 = -6.303$; $d_3 = -0.450$; $d_4 = -3.846$; $T_r = T/518.9$.

Equation (2) was used for obtaining the reference data by regression of the data obtained from those calculated from reference data of solubility of methylcyclopentane in water by the Equation of State with an association term. Comparison between reference and experimental data is one of the criteria used to assign data to the categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 14. All the data are in poor agreement with the reference data and are Doubtful.

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[6] are independent data. Therefore these data are Rejected.

References:

[1]B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).
[2]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).
[3]C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
[4]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[5]E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).
[6]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

TABLE 13. Experimental values for solubility of methylcyclopentane (1) in water (2)

T/K	Experimental values x_1 (R=recommended, D=doubtful)	Reference values $x_1 \pm 30\%$
298.2	$9.00 \cdot 10^{-6}$ (R; Ref. 3), $8.95 \cdot 10^{-6}$ (R; Ref. 4), $9.60 \cdot 10^{-6}$ (R; Ref. 5)	$1.0 \cdot 10^{-5}$
334.7	$4.90 \cdot 10^{-5}$ (D; Ref.2)	$1.3 \cdot 10^{-5}$
419.2	$3.31 \cdot 10^{-4}$ (D; Ref.2)	$7.5 \cdot 10^{-5}$
457.2	$9.76 \cdot 10^{-4}$ (D; Ref.2)	$2.1 \cdot 10^{-4}$
487.2	$3.15 \cdot 10^{-3}$ (D; Ref.2)	$5.2 \cdot 10^{-4}$

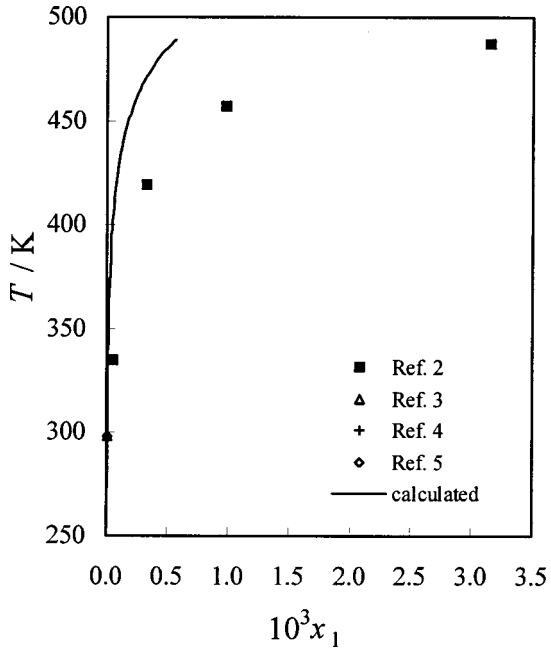

FIG. 7. All the solubility data for methylcyclopentane (1) in water (2).

TABLE 14. Experimental values for solubility of water (2) in methylcyclopentane (1)

T/K	Experimental values x_2 (D=doubtful)	Reference values $x_2 \pm 30\%$
283.2	$3.40 \cdot 10^{-4}$ (D; Ref. 1)	$2.2 \cdot 10^{-4}$
293.2	$6.12 \cdot 10^{-4}$ (D; Ref. 1)	$3.6 \cdot 10^{-4}$
303.2	$9.58 \cdot 10^{-4}$ (D; Ref. 1)	$5.7 \cdot 10^{-4}$

Components:
(1) Methylcyclopentane; C_6H_{12} ; [96-37-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
Temperature: 10 °C–30 °C

Prepared By:
A. Maczynski and M. C. Haulait-Pirson

Experimental Data
Solubility of water in methylcyclopentane

t/°C	$10^4 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	3.4	0.073
20	6.12	0.0131
30	9.58	0.0205

Auxiliary Information

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

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

Estimated Error:
Not specified.

Components:
(1) Methylcyclopentane; C_6H_{12} ; [96-37-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **19**, 77 (1964).

Variables:
Temperature: 61.5 °C–214 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

Solubility of methylcyclopentane in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g(2)	$g(1)$/100 g sln (compiler)
61.5	0.490	0.0229	0.0229
146	3.31	0.155	0.155
184	9.76	0.457	0.457
214	31.20	1.479	1.457

Auxiliary Information

Method/Apparatus/Procedure:
Presumably the measurements were made in sealed glass tubes, as reported in Guseva and Parnov.[1] No more details were reported in the paper.

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

Estimated Error:
Not specified.

References:
[1]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).

Components:
(1) Methylcyclopentane; C_6H_{12} ; [96-37-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of methylcyclopentane in water at 25 °C was reported to be 42 mg(1)/kg sln.
The corresponding mole fraction, x_1, calculated by the compiler, is $9.0 \cdot 10^{-6}$.
The same value is also reported in McAuliffe.[1,2]

Auxiliary Information

Method/Apparatus/Procedure:
In a 250-mL glass bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 L sample of the hydrocarbon-saturated water was withdrawn with a Hamilton Syringe and injected into a gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

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

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 1.6 mg(1)/kg sln (standard deviation from mean).

References:
[1]C. McAuliffe, Nature (London) **200**, 1092 (1963).
[2]C. McAuliffe, Am. Chem. Soc. Div. Petrol. Chem. **9**, 275 (1964).

Components:
(1) Methylcyclopentane; C_6H_{12} ; [96-37-7]
(2) Water; H_2O; [7732-18-5]

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

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of methylcyclopentane in water at 25 °C and at the system pressure was reported to be 41.8 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00418 $g(1)$/100 g sln and $8.95 \cdot 10^{-6}$.

Auxiliary Information

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

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

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

Components:
(1) Methylcyclopentane; C_6H_{12} ; [96-37-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. S. Rudakov and A. I. Lutsyk, Zh. Fiz. Khim. **53**, 1298 (1979).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The authors reported the partition coefficient α of methylcyclopentane between the gas and aqueous phase. $\alpha = 14 \pm 1$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25 °C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of P (where P is the vapor pressure in mm of Hg) is taken from Hine and Mooker.[1] $P = 137.5$ mm of Hg and $\log C_g = \log P - 4.269 = -2.13$ expressed in moles per liter. Therefore $C_s = 5.29 \cdot 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g·mL, the corresponding mass percent is 0.0045 $g(1)$/100 g sln and the corresponding mole fraction, x_1, is $9.6 \cdot 10^{-6}$.

Auxiliary Information

Method/Apparatus/Procedure:
The equilibrium distribution was attained after shaking for 10 min a thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and the solution were introduced by a syringe into a special cell for the removal of (1) by sparging, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.

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

Estimated Error:
Solubility: ±10% (estimated by the compiler).

References:
[1] J. Hine and P. K. Mooker, J. Org. Chem. **4**, 292 (1975).

3.10. 2-Methyl-1-pentene

Components:	Original Measurements:
(1) 2-Methyl-1-pentene; C_6H_{12} ; [763-29-1] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of 2-methyl-1-pentene in water at 25 °C was reported to be 78 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0078 $g(1)$/100 g sln and $1.7 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C
Solubility: 3.2 mg(1)/kg(2) (standard deviation of mean).

3.11. 4-Methyl-1-pentene

Components:	Original Measurements:
(1) 4-Methyl-1-pentene; C_6H_{12} ; [691-37-2] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of 4-methyl-1-pentene in water at 25 °C was reported to be 48 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0048 $g(1)$/100 g sln and $1.0 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250-mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ±1.5 °C.
Solubility: 2.6 mg(1)/kg(2) (standard deviation of mean).

4. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

5. Registry Number Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

6. Author Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.