COMPONENTS:	EVALUATOR:
(1) Cyclohexene; C_6H_{10}; [110-83-8]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia.
(2) Water; H_2O; [7732-18-5]	November 1984.

CRITICAL EVALUATION:

Quantitative solubility data for the system cyclohexene (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Cyclohexene (1) - Water (2) System

Reference	T/K	Solubility	Method
McBain and Lissant (ref 1)	298	(1) in (2)	synthetic
Duque-Estrada *et al.* (ref 2)	298	(1) in (2)	GLC
Englin *et al.* (ref 3)	283-313	(2) in (1)	analytical
Farkas (ref 4)	298	(1) in (2)	GLC
McAuliffe (ref 5)	298	(1) in (2)	GLC
Pierotti and Liabastre (ref 6)	278-318	(1) in (2)	GLC
Budantseva *et al.* (ref 7)	293	mutual	GLC, Karl Fischer
Schwarz (ref 8)	297	(1) in (2)	chromatographic

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Solubilities of cyclohexene in various aqueous salt solutions have also been reported (ref 9) but will not be considered in this Evaluation. For convenience, further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF CYCLOHEXENE (1) IN WATER (2)

The solubility data for cyclohexene in water are listed in Table 2. There are too few values to justify plotting them in a Figure.

At 298 K, the results of Pierotti and Liabastre (ref 6) appear to be much higher than all other values. This situation is typical of the large number of hydrocarbon-water systems investigated by these authors and is discussed in greater detail in the Critical Evaluation for the cyclopentane-water system. On the other hand, Pierotti and Liabastre's results at other temperatures are in reasonable agreement with the other available data (ref 7,8). This probably means that these data are also higher than "true" values. However, in the absence of confirmatory studies it is not possible to reject these data (ref 6,7,8). They are included in Table 2 but excluded in the determination of "Best" values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Cyclohexene; C_6H_{10}; [110-83-8]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia.
(2) Water; H_2O; [7732-18-5]	November 1984.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Value of the Solubility of Cyclohexene (1) in Water (2)

T/K	Solubility values		
	Reported values g(1)/100g sln	"Best" value g(1)/100g sln	$(\pm \sigma_n)^a$ $10^5 x_1$
278	0.028 (ref 6)		
288	0.029 (ref 6)		
293	0.023 (ref 4)		
298	0.013 (ref 1), 0.014 (ref 2), 0.016 (ref 4), 0.0213 (ref 5), 0.030 (ref 6), 0.028[b] (ref 8)	0.016 ± 0.003	3.5
308	0.030 (ref 6)		
318	0.031 (ref 6)		

a Obtained by averaging reported values excluding those of ref 6 (see text) and ref 8 (297K datum). σ_n values do not have statistical significance.

b 297 K datum.

2. THE SOLUBILITY OF WATER (2) IN CYCLOHEXENE (1)

The solubility data for water in cyclohexene are listed in Table 3. The results of Englin *et al.* (ref 6) and Budantseva *et al.* (ref 7) at 293 K are only in fair agreement.

It should be noted that in a number of well-characterised systems (e.g. benzene-water) the data of Englin *et al.* are usually reliable when T < 300 K but are much higher than "Recommended" values when T > 300 K. Thus, in the absence of confirmatory studies, all the data in Table 3 should be regarded very cautiously.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Cyclohexene; C_6H_{10}; [110-83-8]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia.
(2) Water; H_2O; [7732-18-5]	November 1984.

CRITICAL EVALUATION: (continued)

TABLE 3: Tentative Solubility Values of Water (2) in Cyclohexene (1)

	Solubility values		
	Reported values	"Best" values ($\pm \sigma_n$)[a]	
	10^2g(2)/100g sln	10^2g(2)/100g sln	$10^3 x_2$
283	2.52 (ref 3)	2.5	1.2
293	3.17 (ref 3), 4.2 (ref 7)	3.7 ± 0.5	1.7
298	3.70[b] (ref 3)	3.7	1.7
303	4.24 (ref 3)	4.2	1.9
313	5.62 (ref 3)	5.6	2.6

a See text, however; σ_n has no statistical significance.

b Interpolated graphically by the Evaluator.

REFERENCES

1. McBain, J.W.; Lissant, K.J. *J. Phys. Chem.* 1951, *55*, 655-62.
2. Duque-Estrada, E.; Bayne, A.H.; Manakan, D.A. Instr. Lab. Rept., Dept. Chem. Eng. MIT, April 22, 1964. (*cf.* ref 4).
3. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
4. Farkas, E.J. *Anal. Chem.* 1965, *37*, 1173-5.
5. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
6. Pierotti, R.A.; Liabastre, A.A. *Structure and properties of water solutions.* U.S. Nat. Tech. Inform. Serv., PB Rep. 1972, No. 21163, 113 pp.
7. Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344; Deposited Doc. 1976, VINITI 438-76.
8. Schwarz, F.P. *Anal. Chem.* 1980, *52*, 10-15.
9. Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	McBain, J.W.; Lissant, K.J. *J. Phys. Colloid. Chem.* 1951, *55*, 665-62.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

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^{-1}), are 0.013 g(1)/100 g sln and 2.9×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL portions 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 solubilized.	(1) Eastman No. 1043. (2) distilled and boiled to remove CO_2.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Duque-Estrada, E.; Bayne, A.H.; Manalan, D.A. Instr. Lab. Rept., Dept. Chem. Eng., MIT, April 22, 1964.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

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 3.1×10^{-5}.

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

The data are taken from ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical (glc) method was used. Nothing more was reported in ref 1.	(1) not specified in ref 1. (2) not specified in ref 1.
	ESTIMATED ERROR: not specified in ref 1.
	REFERENCES: 1. Farkas, E.J. *Anal. Chem.* 1965, *37*, 1173.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
VARIABLES:	**PREPARED BY:**
Temperature: 10-40°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in cyclohexene

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. 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.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Farkas, E.J. *Anal. Chem.* 1965, *37*, 1173-5.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and A. Szafranski

EXPERIMENTAL VALUES:

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} sln.

The corresponding temperature, mass percent, and mole fraction, x_1, calculated by compilers at 25°C, 0.016 g(1)/100 g sln, and 3.5×10^{-5}. The assumption that 1 ft^3 sln = 28.32 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. ± 6% (mean from three determinations) (compiler)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of cyclohexene in water at 25°C was reported to be 213 g(1)/10^6 g(2).
The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0213 g(1)/100 g sln and 4.67×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, 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:

temp. ± 1.5 K
soly. 10 g(1)/10^6 g(2) (standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9
VARIABLES:	PREPARED BY:
One temperature 30°C	M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of cyclohexene in water was reported to be 4.950×10^{-3} mol L^{-1} at 30°C.[a] Assuming a solution density of 1.00 g mL^{-1} the corresponding mass percent and mole fraction (x_1) solubilities calculated by the compilers are respectively, 0.0406 g(1)/100 g sln and 8.91×10^{-5}.

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

[a] 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^{-1} HNO_3 solution.

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 olefin content determined by titration with bromine using standard procedures.	(1) Prepared by dehydration of cyclohexanol and then washed, dried and fractionated. Purity (no specification) was determined by chromatography. (2) Not specified.
	ESTIMATED ERROR: Temp. ± 0.05 K Soly. not specified
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., 1972, No. 21163, 113 p.
VARIABLES:	PREPARED BY:
Temperature: 278.26-318.36 K	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclohexene in water

T/K	g(1)/100 g sln	$10^3 x_1$
278.26	0.02800 ± 0.00069	0.06141
288.36	0.02985 ± 0.00061	0.06546
298.26	0.02990 ± 0.00082	0.06557
308.36	0.03025 ± 0.00070	0.06634
318.36	0.03105 ± 0.00093	0.06809

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 the rotating basket and rotated for 24 hours. 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 hours. 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) Eastman Organic Chemicals, No. 1043; washed with water to remove stabilizing agent.

(2) laboratory distilled water.

ESTIMATED ERROR:

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

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344. *Deposited doc.* 1976, VINITI 438-76.
VARIABLES:	**PREPARED BY:**
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

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

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:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by Karl Fischer reagent method.	(1) source not specified; pure or analytical reagent grade; purity <99.9%. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Schwarz, F.P. *Anal. Chem.* 1980, *52*, 10-15.
VARIABLES:	**PREPARED BY:**
One temperature: 23.5°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclohexene in water at 23.5°C

g(1)/100 g sln	$10^5 x_1$ (compiler)
0.0281 ± 0.0005	6.16
0.0286 ± 0.0013	6.27

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 (ca. 14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e. length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) reagent grade used without further purification

(2) distilled

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 3% (average std. dev.)

REFERENCES: