COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]	G.T. Hefter, School of Mathematical
(2) Water; H <sub>2</sub> O; [7732-18-5]	and Physical Sciences, Murdoch
	University, Perth, W.A., Australia.
	September 1986.

### CRITICAL EVALUATION:

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

TABLE 1: Quantitatuve Solubility Studies of the Cyclohexane(1) - Water (2) System

Berkengeim (ref 3)  Black et al. (ref 4)  Durand (ref 5)  McBain and Lissant (ref 6)	T/K 290 287-326 293-323 293 289 298	Solubility (1) in (2) (2) in (1) (2) in (1) (2) in (1) (1) in (2)	Method volumetric synthetic Karl Fischer radiotracer
Tarassenkow and Poloshinzewa (ref 2)  Berkengeim (ref 3)  Black et al. (ref 4)  Durand (ref 5)  McBain and Lissant (ref 6)  Kudchadker and McKetta	287-326 293-323 293 289	(2) in (1) (2) in (1) (2) in (1)	synthetic Karl Fischer radiotracer
Poloshinzewa (ref 2) Berkengeim (ref 3) Black et al. (ref 4) Durand (ref 5) McBain and Lissant (ref 6) Kudchadker and McKetta	293-323 293 289	(2) in (1) (2) in (1)	Karl Fischer radiotracer
Black et al. (ref 4) Durand (ref 5) McBain and Lissant (ref 6) Kudchadker and McKetta	293 289	(2) in (1)	radiotracer
Durand (ref 5) McBain and Lissant (ref 6) Kudchadker and McKetta	289		
McBain and Lissant (ref 6) Kudchadker and McKetta		(1) in (2)	
Kudchadker and McKetta	298	• • • • •	cloud point
		(1) in (2)	cloud point
	311-411 <sup>a</sup>	(1) in (2)	not specified
Guseva and Parnov (ref 9,10)	298-494	(1) in (2)	synthetic
Englin $et$ $al$ . (ref 11)	289-323	(2) in (1)	analytical
Zel'venskii <i>et al</i> . (ref 12)	293	(2) in (1)	radiotracer
Johnson $et$ $al.$ (ref 13)	298	(2) in (1)	Karl Fischer
McAuliffe (ref 14)	298	(1) in (2)	GLC
Gregory et al. (ref 15)	298	(2) in (1)	Karl Fischer
Rebert and Hayworth (ref 8,16)	403-643 <sup>a</sup>	mutual	synthetic
Burd and Braun (ref 17)	368-478 <sup>a</sup>	(2) in (1)	GLC
Bröllos <i>et al</i> . (ref 18)	275-421 <sup>a</sup>	mutual	synthetic
Roddy and Coleman (ref 19)	298	(2) in (1)	radiotracer
Roof (ref 20)	530	mutual	synthetic
Plenkina $et$ $al$ . (ref 21)	403-523	(2) in (1)	synthetic
Glasoe and Schultz (ref 22)	288-303	(2) in (1)	Karl Fischer
Pierotti and Liabastre (ref 23)	278-318	(1) in (2)	GLC
Leinonen and Mackay (ref 24)	298	(1) in (2)	GLC
Sultanov and Skripka (ref 25,32)	473-523 <sup>a</sup>	(2) in (1)	not specified
Goldman (ref 26)	283-313	(2) in (1)	Karl Fischer
Mackay <i>et al</i> . (ref 27,28)	298	(1) in (2)	GLC
Budantseva <i>et al</i> . (ref 29)	293	mutual	GLC, Karl Fischer
Kirchnerova and Cave (ref 30)	298	(2) in (1)	Karl Fischer
Price (ref 31)	298	(1) in (2)	GLC

COMP	ONENTS:		
(1)	Cyclohexane;	C <sub>6</sub> H <sub>12</sub> :	[110-82-7]
(2)	Water; H <sub>2</sub> O;	[7732-18	3-5]

### EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A. Australia. September 1986.

### CRITICAL EVALUATION:

### TABLE 1 (continued)

<del>                                   </del>			i
Reference	T/K	Solubility	Method
Korenman and Aref'eva (ref 33)	293,298	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 35)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 36)	298	(1) in (2)	partition coefficient
Schwarz (ref 37)	297	(1) in (2)	chromatographic
Tsonopoulos and Wilson (ref 39)	313-482 <sup>a</sup>	mutual	GLC, Karl Fischer

<sup>&</sup>lt;sup>a</sup>Pressure also varied, see Table 4

Solubility data for cyclohexane in water may also be calculated from the calorimetric data of Gill  $et\ al$ . (ref 40) and quantitative solubility data for the cyclohexane-heavy water (D<sub>2</sub>O) system are given in the publications of Guseva and Parnov (ref 9) and Backx and Goldman (ref 38).

Apart from the paper by Roof (ref 20), which did not contain sufficient information to justify compilation, the original data in all the publications listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation. The datum of Krzyzanowska and Szeliga (ref 35) does not appear to be indendent of that of Price (ref 31) and so has been excluded from this Evaluation.

Despite the large number of investigations of this system (Table 1), the mutual solubilities are poorly characterised and warrant thorough reinvestigation over the entire liquid range. No data have been "Recommended".

In the Tables which follow values which have been obtained by the Evaluator by graphical interpolation of the original data are indicated by an asterisk (\*). "Best" values were obtained by simple averaging. The uncertainty limits  $(\sigma_n)$  attached to these values do not have statistical significance and should be regarded only as convenient representation of the spread of reported values rather than error limits.

For convenience, further discussion of this system will be divided into three sections.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7] (2) Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

1. THE SOLUBILITY OF CYCLOHEXANE (1) IN WATER (2)
Most of the available data for the solubility of cyclohexane in water are
summarized in Table 2 below.

In preparing Table 2 below the data of Mackay et al. (ref 27) were excluded as the temperature was not specified; anyway, these data are probably superceded by later measurements from the same laboratory (ref 28). The various data reported at high temperature have also been excluded as they are discussed in detail in section 3 below. The datum of Schwarz (ref 37) at 296.7K, although in reasonable agreement with other values, has been excluded for representational convenience.

At 298K, the only temperature where sufficient data have been obtained to enable meaningful evaluation to be made, the approximate values of Guseva and Parnov (ref 9,10) and Korenman and Aref'eva are rejected as is the datum of Pierotti and Liabastre (ref 23) which is markedly higher than all other values. All other data are included in Table 2.

At other temperatures the data are much too scattered to enable a satisfactory evaluation to be made. This can be clearly seen from Figure 1 which plots all the available data. Thus no "Best" values have been calculated in Table 2 other than at 298K. Clearly, this system requires a thorough reinvestigation over the whole temperature range.

TABLE 2: Solubility of Cyclohexane (1) in Water (2)

	Solubility	values	
T/K	Reported values 10 <sup>3</sup> g(1)/100 g sln	"Best" value (± σ <sub>n</sub> ) <sup>α</sup> 10 <sup>3</sup> g(1)/100 g sln	10 <sup>5</sup> x <sub>1</sub>
278	8.19 (ref 23)		
288	$6.2^{b}$ (ref 5), 8.87 (ref 23)		
293	7.0 (ref 29) 10 (ref 33)		
298	5.5 (ref 14), 5.67 (ref 24), 5.75 (ref 28), 6.65 (ref 31), 5.5 (ref 36)	5.8 ± 0.4	1.2
308	4.54 <sup>c</sup> (ref 7), 8.88 (ref 23)		
318	9.13 (ref 23), 7.14* (ref 39)		
323	7.55 (ref 39)		
329	17 (ref 9,10)		
343	10.1 (ref 39)		
344	2.7 (ref 7)		

a Best values not calculated except at 298 K (see text)

b Refers to 289K

c Refers to 310K (continued next page)

- (1) Cyclohexane;  $C_{6}^{H}_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

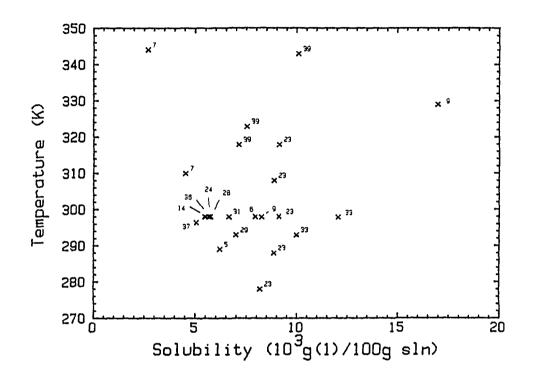


FIGURE 1. Solubility data for cyclohexane (1) in water. Numbers refer to the reference list. No line of best fit plotted because of scatter in data.

### 2. THE SOLUBILITY OF WATER (2) IN CYCLOHEXANE (1)

There are more solubility data for the hydrocarbon-rich phase than for the water-rich phase. Although the values of Tarassenkow and Poloshinzewa (ref 2) and Englin et al. (ref 11) are in good agreement over a wide temperature range, they are approximately twice as large as those reported by Goldman (ref 26) which in turn are close to those of most other studies (see Table 3). It should also be noted that the solubility data reported in ref 2 and ref 11 for a number of well-defined hydrocarbon-water systems are significantly higher than "Recommended" values. Nevertheless, there are insufficient independent data at present to justify exclusion of any values and thus all results are included in Table 3. In view of the lack of agreement between the various studies, the averaged "Best" values should be regarded as very tentative.

(continued next page)

- (1) Cyclohexane;  $C_{6}H_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### **EVALUATOR:**

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

TABLE 3: Solubility of Water (2) in Cyclohexane (1)

T/K	Solubili	ty values	
	Reported values	"Best" values	
	10 <sup>3</sup> g(2)/100g sln	10 <sup>3</sup> g(2)/100g sln	· $10^4 x_2$
283	4* (ref 2), 6.7 (ref 11), 3.4 (ref 2)	5 ± 1	2.3
293	9* (ref 2), 8.7 (ref 3), 10 (ref 4), 12.2 (ref 11), 9.8 (ref 12), 5.9 (ref 26), 10.1 (ref 29)	9 ± 2	4.2
298	<pre>13* (ref 2), 5.6 (ref 13), 6.9 (ref 15), 8.0 (ref 19), 7.4 (ref 22), 7.0 (ref 26), 7.0 (ref 30)</pre>	8 ± 2	3.7
303	17* (ref 2), 19.4 (ref 11), 8.7 (ref 22), 9.6 (ref 26)	14 ± 5	6.5
313	31* (ref 2), 31.7 (ref 11), 13.1 (ref 26), 13.3 (ref 39)	24 ± 8	12
323	46* (ref 2), 15 (ref 3), 49 (ref 11), 19.4* (ref 39)	32 ± 15	17

The data in Table 3 are also plotted in Figure 2. This plot shows that the temperature dependence of the solubility observed by Goldman (ref 26) and Glasoe and Schultz (ref 22) is much less than that of ref 2 and ref 11.

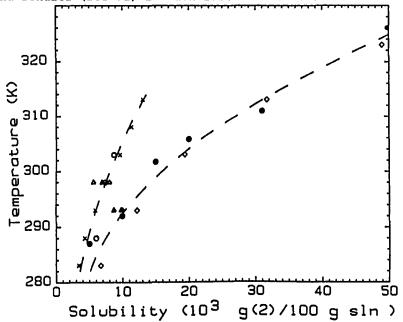


FIGURE 2. Solubility of water in cyclohexane: ref 2 ( $\bullet$ ); ref 11 ( $\diamond$ ); ref 22 ( $\circ$ ); ref 26 (x); other data ( $\Delta$ ). Full lines not drawn through data points because of poor agreement (see text). (continued)

COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7] (2) Water; H <sub>2</sub> O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia.
	September 1986.

CRITICAL EVALUATION: (continued)

3. THE MUTUAL SOLUBILITIES OF CYCLOHEXANE (1) AND WATER (2) AT ELEVATED PRESSURES

To clarify the relationship between the phases in equilibrium it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram. Cyclohexane + water exhibits type III phase behaviour (ref 41,42) and the projection is topographically similar to that of benzene + water.

Solubilities in the cyclohexane-water system have been studied at higher than atmospheric pressures in the publications listed in Table 4.

TABLE 4: Solubility Studies of the Cyclohexane-Water
System at Elevated Pressures

p/MPa	T/K	Solubility
0.1-3	311-411	(1) in (2)
_a	298-493	(1) in (2)
0.6-22.1	403-643	mutual
0.2-3	368-478	(2) in (1)
19-174	275-421	mutual
<b>-</b> <sup>D</sup>	- <sup>D</sup>	<b>-</b> <sup>b</sup>
<b>-</b> <sup>a</sup>	403-523	(2) in (1)
3-79	473-523	(2) in (1)
0.3-3	313-482	mutual
	0.1-3 -a 0.6-22.1 0.2-3 19-174 -b -a 3-79	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

a Along three phase line

In view of the limited amount of data at high pressures and the differing conditions employed, no Critical Evaluation is possible at present. However, the solubilities of water in cyclohexane at  $p \cong 3$  MPa,  $T \approx 473$ K reported by Burd and Braun (ref 17) and Sultanov and Skripka (ref 25,32) are in reasonable agreement (approximately 3.0 and 3.8 g(2)/100 g sln respectively) but differ significantly from that reported by Tsonopoulos and Wilson (ref 39), (1.7 g(2)/100 g sln). Similarly, the atmospheric pressure data of Kudchadker and McKetta (ref 7) are only in fair agreement with comparable data (Table 3). Their conclusion that the solubility of cyclohexane in water increases linearly with pressure at a given temperature is inconsistent with the results for numerous hydrocarbon-water systems as noted by Guseva and Parnov (ref 9,10).

(continued next page)

b Critical point at unspecified composition

- (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### **EVALUATOR:**

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. September 1986.

CRITICAL EVALUATION: (continued)

The temperature and pressure of the critical end point have been determined by Rebert and Hayworth (ref 8,16) and by Roof (ref 20). The values are in good agreement.

Reference	T/K	p/MPa
Rebert and Hayworth (ref 8,16)	528.9	8.019
Roof (ref 20)	529.9	8.039

Bröllos et al. (ref 18) have reported detailed measurements in the high pressure region between the critical temperatures of the pure components. These data are for the two phase-one phase boundary and at most pressures and temperatures studied the phases are at liquid-like densities. These data are probably reliable as they were determined using a reliable, well-tested experimental method. However, in the absence of confirmatory studies no Critical Evaluation is possible.

The interested user is referred to the original measurements compiled in the data sheets following this Critical Evaluation for experimental values.

### REFERENCES

- 1. Bennett, G.M.; Philip, W.G. J. Chem. Soc. 1928, 1937-42.
- 2. Tarassenkow, D.N.; Poloshinzewa, E.N. Chem. Ber. 1932, 65, 184-6.
- 3. Berkengeim, T.I. Zavod. Lab. 1941, 10, 592-4.
- 4. Black, C.; Joris, G.G.; Taylor, H.S. J. Chem. Phys. <u>1948</u>, 16, 537-43.
- 5. Durand, R. C.R. Hebd. Seances Acad. Sci. 1948, 226 409-10.
- 6. McBain, J.W.; Lissant, K.J. J. Phys. Chem. 1951, 55, 655-62.
- Kudchadker, A.P.; McKetta, J.J. A.I.Ch.E.J. 1961, 7, 707.
- Hayworth, K.E.; M.S. Thesis, 1962, Univ. Southern California, Los Angeles (U.S.A.), quoted in ref 16.
- Guseva, A.N.; Parnov, E.I. Radiokhimiya <u>1963</u>, 5, 507-9.
- 10. Guseva, A.N.; Parnov, E.I. Zh. Fiz. Khim. 1963, 37, 2763.
- Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. Khim. Tekhnol. Topl. Masel 1965, 10, 42-6.
- Zel'venskii, Ya.D.; Egremov, A.A.; Larin, G.M. Khim. Tekhnol. Topl. Masel 1965 10, 3-7.
- Johnson, J.R.; Christian, S.D.; Affsprung, H.E. J. Chem. Soc. A 1966, 77-8.
- 14. McAuliffe, C. J. Phys. Chem. 1966, 70, 1267-75.

<u>(continued next page)</u>

- (1) Cyclohexane;  $C_{6}H_{12}$ ; [1100-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### **EVALUATOR:**

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

### REFERENCES (continued)

- 15. Gregory, M.D.; Christian, S.D.; Affsprung, H.E. J. Phys. Chem. 1967, 71, 2283-9.
- 16. Rebert, C.J.; Hayworth, K.E. A.I.Ch.E.J. 1967, 13, 118-21.
- Burd, Jr., S.D.; Braun, W.G. Proc. Div. Refining, Amer. Petrol. Inst. 1968, 48, 464-76.
- 18. Bröllos, K.; Peter, K.; Schneider, G.M. Ber. Bunsenges. Phys. Chem. 1970, 74, 682-6.
- 19. Roddy, J.W.; Coleman, C.F. Talanta 1968, 15, 1281-6.
- 20. Roof, J.G. J. Chem. Eng. Data 1970, 15, 301-3.
- Plenkina, R.M.; Pryanikova, R.O.; Efremova, G.D.; Deposited Doc. VINITI 3028-71; Zh. Fiz. Khim. 1971, 45, 2389.
- 22. Glasoe, P.K.; Schultz, S.D. J. Chem. Eng. Data 1972, 17, 66-8.
- Pierotti, R.A.; Liabastre, A.A.; U.S. Nat. Tech. Inform. Serv., PB rep. 1972, Mo.21163, 113 pp.
- 24. Leinonen, P.J.; Mackay, D. Can. J. Chem. Eng. 1973, 51, 230-3.
- Sultanov, R.G.; Skripka, V.G.; Deposited Doc. VINITI 5347-72; Zh. Fiz. Khim. 1973, 40, 1035.
- 26. Goldman, S. Can. J. Chem. 1974, 52, 1668-80.
- Mackay, D.; Shiu, W.Y.; Wolkoff, A.W. Water Quality Parameters, ASTM STP 573, 1975, 251.
- 28. Mackay, D.; Shiu, W.Y. Can. J. Chem. Eng. 1975, 53, 239-41.
- 29. Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. Deposited Doc. VINITI 438-76; Zh. Fiz. Khim. 1976, 50, 1343.
- 30. Kirchnerova, J.; Cave, G.C.B. Can. J. Chem. 1975, 54, 3909-16.
- 31. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
- 32. Skripka, V.A. Tr. Vses. Neftegazov. Nauch Issled. Inst. <u>1976</u>, 61, 139-51.
- Korenman, I.M.; Aref'eva, R.P.; Patent USSR, 553 524, 1977, 04.05.
   C.A. 87:87654.
- 34. Korenman, I.M.; Aref'eva, R.P. Zh. Prikl. Khim. 1978, 51, 957-8.
- 35. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7.
- 36. Rudakov, E.S.; Lutsyk, A.I. Zh. Fiz. Khim. 1979, 53, 1298-1300.
- 37. Schwarz, F.P. Anal. Chem. 1980, 52, 10-15.
- 38. Backx, P.; Goldman, S. J. Phys. Chem. 1981, 85, 2975-9.

(continued next page)

- (1) Cyclohexane;  $C_{6}H_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

### REFERENCES (continued)

- 39. Tsonopoulos, C.; Wilson, G.M. A.I.Ch.E.J. 1983, 29, 990-9.
- 40. Gill, S.J.; Nichols, N.F.; Wadso, I. J. Chem. Thermodyn. 1976, β, 445-52; and references cited therein.
- Scott, R.L.; van Konynburg, P.H. Phil. Trans. Roy. Soc., London 1980, A298, 495.
- 42. Hicks, C.P.; Young, C.L. Chem. Rev. 1975, 75, 119.

### ACKNOWLEDGEMENTS

The Evaluator thanks Dr Brian Clare for the regression analyses and graphics and Dr Marie-Claire Haulait-Pirson for comments and a preliminary draft of the reference list. Section 3 was written jointly with C. L. Young, Department of Physical Chemistry, University of Melbourne, Australia.

### COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] (2) Water; H<sub>2</sub>O; [7732-18-5] VARIABLES: Temperature: 14-53°C ORIGINAL MEASUREMENTS: Tarassenkow, D.N.; Poloshinzewa, E.N. Ber. Dtsch. Chem. Ges. 1932, 65B, 184-6.

### EXPERIMENTAL VALUES:

### Solubility of water in cyclohexane

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

### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No details were reported in the paper.	(1) Kahlbaum; dried over calcium chloride and twice distilled over Na-K.
	(2) not specified.
	ESTIMATED ERROR:
	soly. ± 0.01%
	REFERENCES:

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Berkengeim, T.I. (2) Water; H<sub>2</sub>O; [7732-18-5] Zavod. Lab. 1941, 41, 592-4. VARIABLES: PREPARED BY: Temperature: 20 and 50°C A. Maczynski

### EXPERIMENTAL VALUES:

### Solubility of Water in Cyclohexane

t/°C	g(2)/100 gsln	10 <sup>4</sup> x <sub>2</sub> (compiler)
20	0.0087	4.1
50	0.015	7.0
30	0.025	, , ,

AUXILIARY INFORMATION						
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:					
The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	(1) source not specified; CP reagent; b.p. 80°C; used as received.					
	(2) not specified.					
	ESTIMATED ERROR:					
	mot specified.					
	REFERENCES:					

- (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Black, C.; Joris, G.G.; Taylor, H.S.

J. Chem. Phys. 1948, 16, 537-43.

### VARIABLES:

PREPARED BY:

One temperature: 20°C

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

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 x  $10^{-4}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The method described in ref 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

(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:

soly. a few percent (type of error
not specified).

### REFERENCES;

1. Joris, G.G.; Taylor, H.S. J. Chem. Phys. 1948, 16, 45.

## COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] (2) Water; H<sub>2</sub>O; [7734-18-5] VARIABLES: One temperature: 16°C ORIGINAL MEASUREMENTS: Durand, R. C.R. Hebd. Seances Acad. Sci. 1948, 226, 409-10.

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at  $16^{\circ}$ C was reported to be  $0.08 \text{ cm}^3(1)/\text{dm}^3(2)$ .

With the assumption of a solution density of 1.00 g cm<sup>-3</sup> and a density value of 0.782 g cm<sup>-3</sup> for cyclohexane at  $16^{\circ}$ C (ref 2), the corresponding mass percent is 0.0062 g(1)/100 g sln and the corresponding mole fraction,  $x_1$ , is 1.3 x  $10^{-5}$  (compiler).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

in ref 1 was used.
Addition of pipetted volumes of
(1) to (2) followed by shaking is
repeated till appearance of
turbidity.

The thermostatic method described

### SOURCE AND PURITY OF MATERIALS:

- (1) not specified
- (2) distilled

### ESTIMATED ERROR:

soly.  $\pm 0.005 \text{ cm}^3(1)/\text{dm}^3(2)$ 

- Durand, R. C.R. Hebd. Seances Acad. Sci. 1946, 223, 898.
- 2. Timmermans, J. Physico-chemical constants of pure organic compounds, Elsevier. 1950.

### 234 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Cyclohexane; $C_{6}H_{12}$ ; [110-82-7] McBain, J.W.; Lissant, K.J. (2) Water; H<sub>2</sub>O; [7732-18-5] J. Phys. Colloid. Chem. 1951, 55, 655-62. VARIABLES: PREPARED BY: M.C. Haulait-Pirson One temperature: 25°C EXPERIMENTAL VALUES: 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 $\,\mathrm{cm}^{-3}$ , the corresponding mass percent is 0.008 g(1)/100 g sln and the corresponding mole fraction, $x_1$ , is 1.7 x $10^{-5}$ (compiler). AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 10 mL of (2) was pipetted into glass (1) C.P. grade. vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials (2) distilled and boiled to remove co2. 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. ESTIMATED ERROR: not specified. REFERENCES:

# COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Kudchadker, A.P.; McKetta, J.J. (2) Water; H<sub>2</sub>O; [7732-18-5] A.I.Ch.E.J. 1961, 7, 707. VARIABLES: Temperature: 100-280°F Pressure: 14.7-450 psia PREPARED BY: M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

Solubility of cyclohexane in water. Smoothed data

			0°F (310.93 K)		0°F (344.26 K)
p/psia	<pre>p/MPa (compiler)</pre>	10 <sup>5</sup> x <sub>1</sub>	g(1)/100 g sln (compiler)	$\frac{10^5 x_1}{}$	g(1)/100 g sln (compiler)
14.7 20.0 30.0 40.0 50.0 60.0 80.0 100.0 120.0	0.101 0.138 0.207 0.276 0.345 0.414 0.552 0.689 0.827 0.965	0.97 1.34 2.03 2.72 3.41 4.10 5.48 6.85 8.22 9.60	0.00454 0.00626 0.00949 0.01272 0.01594 0.01917 0.02562 0.03202 0.03842 0.04487	0.58 1.00 1.60 2.20 2.93 3.45 4.71 5.92 7.18 8.43	0.00271 0.00468 0.00748 0.01029 0.01323 0.01613 0.02202 0.02767 0.03356 0.03940
160.0 180.0 200.0 250.0 300.0 350.0 400.0	1.103 1.241 1.379 1.724 2.068 2.413 2.758 3.103	11.03 12.04 13.8 17.08 20.2 23.11 25.84 28.35	0.05155 0.05627 0.06449 0.07981 0.09438 0.10796 0.12070	9.71 10.92 12.28 15.41 18.24 21.0 23.61 25.98	0.04538 0.05104 0.05739 0.07201 0.08522 0.09811 0.11029 0.12135

(continued)

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The experimental technique and the analytical procedure are described in detail in ref 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:

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

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Kudchadker, A.P.; McKetta, J.J. (2) Water; H<sub>2</sub>O; [7732-18-5] A.I.Ch.E.J. 1961, 7, 707.

### Solubility of cyclohexane in water. Smoothed data

			0°F (377.59 K)	t = 28	0°F (410.93 K)
p/psia	<pre>p/MPa (compiler)</pre>	10 <sup>5</sup> x <sub>1</sub>	g(1)/100 g sln (compiler)	105x1	g(1)/100 g sln (compiler)
14.7 20.0 30.0 40.0 50.0	0.101 0.138 0.207 0.276 0.345 0.414	0.72 1.32 1.92 2.51	0.00337 0.00617 0.00898 0.01173	0.70	0.00327
80.0 100.0 120.0 140.0 160.0 200.0 250.0	0.552 0.689 0.827 0.965 1.103 1.241 1.379	3.70 4.89 6.05 7.27 8.48 9.69 10.8 13.92	0.01730 0.02286 0.02828 0.03398 0.03964 0.04529 0.05048 0.06505	1.91 3.13 4.40 5.62 6.82 7.95 9.08 12.1	0.00893 0.01463 0.02057 0.02627 0.03188 0.03716 0.04244 0.05655
300.0 350.0 400.0 450.0	2.068 2.413 2.758 3.103	16.68 19.2 21.52 23.46	0.07794 0.08971 0.10054 0.10959	14.6	0.06823

(1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]

(2) Water; H<sub>2</sub>O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Zh. Fiz. Khim. 1963, 37, 2763.

VARIABLES:

PREPARED BY:

Temperature: 25-220.5°C

A. Maczynski

### EXPERIMENTAL VALUES:

### Solubility of cyclohexane in water

t/°C	g(1)/100 g(2)	g(1)/100 g sln	10 <sup>4</sup> x <sub>1</sub> (compiler)
25	0.008	0.008	0.17
56	0.017	0.017	0.36
94	0.028	0.028	0.60
127	0.0517	0.0517	1.11
162	0.146	0.146	3.13
220.5	1.785	1.784	38.72

The same data are reported in ref 1.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined in sealed glass ampules at pressures less than  $17 \text{ kg/cm}^2$ . No more details were reported in the paper.

### SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

### ESTIMATED ERROR:

Not specified.

### REFERENCES:

 Guseva, A.N.; Parnov, E.I. Radiokhimiya 1963, 5, 507-9.

### COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. (2) Water; H<sub>2</sub>O; [7732-18-5] Khim. Tekhnol. Topl. Masel 1965, 10, 42-6. VARIABLES: PREPARED BY:

### EXPERIMENTAL VALUES:

Temperature: 10-50°C

### Solubility of water in cyclohexane

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

A. Maczynski and M.C. Haulait-Pirson

### AUXILIARY INFORMATION

AUXILIANI INFORMATION						
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:					
Component (1) was introduced into a thermostatted flask and saturated for 5 hours 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.					
	REFERENCES:					

# COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] (2) Water, H<sub>2</sub>O; [7732-18-5] VARIABLES: ORIGINAL MEASUREMENTS: Zel'venskii, Ya.D; Efremov, A.A.; Larin, G.M. Khim. Tekhnol. Topl. Masel 1965, 10, 3-7. PREPARED BY: One temperature: 20°C A. Maczynski

### EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at  $20^{\circ}$ C was reported to be 0.0098 g(2)/100 g sln.

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

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Saturated solutions of tritium 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 mL (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 conc. H<sub>2</sub>SO<sub>4</sub> + HNO<sub>3</sub>; washed with water, dried over sodium, and distilled; purity not specified. b.p. 80.82°C.
- (2) source not specified; commercial; l Ci/mL HTO used as received.

### ESTIMATED ERROR:

not specified.

### COMPONENTS: ORIGINAL MEASUREMENTS: Johnson, J.R.; Christian, S.D.; (1) Cyclohexane; $C_6H_{12}$ ; [110-82-7] Affsprung, H.E. (2) Water; H<sub>2</sub>O; [7732-18-5] J. Chem. Soc. A 1966, 77-8. VARIABLES: PREPARED BY: M.C. Haulait-Pirson One temperature: 25°C

### EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 25°C was reported to be  $0.0024 \text{ mol}(2) \text{ dm}^{-3} \text{ sln}.$ 

With the assumption of a solution density of  $0.7739 \text{ g cm}^{-3}$  (density value of pure cyclohexane reported in ref 2), the corresponding mass percent is 0.0056 g(2)/100 g sln and the corresponding mole fraction,  $x_2$ , is 2.6 x  $10^{-4}$  (compiler).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solute isopiestic apparatus described in ref 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-plate oldershaw column.
- (2) not specified.

### ESTIMATED ERROR:

temp. ± 0.1 K soly. ± 0.0003 mol(2) dm<sup>-3</sup> sln (type of error not specified)

- Christian, S.D.; Affsprung, H.E.; Johnson, J.R.; Worley, J.D. J. Chem. Educ. 1963, 40, 419.
   Goldon, S. Can. J. Chem. 1974,
- 52, 1668.

- (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, 70, 1267-75.

### VARIABLES:

PREPARED BY:

One temperature: 25°C

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at  $25\,^{\circ}\text{C}$  was reported to be  $55\,\text{mg}$  (1)/kg sln.

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

The same value is also reported in refs 1 and 2.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

In a 250 mL glass 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. 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 A 50 μL checked microscopically. sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the 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:

temp. ± 1.5 K

- McAuliffe, C. Nature (London) 1963, 200, 1092.
- McAuliffe, C. Am. Chem. Soc. Div. Petrol. Chem. 1964, 9, 275.

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Gregory, M.D.; Christian, S.D.; Affsprung, H.E. (2) Water; H<sub>2</sub>O; [7732-18-5] J. Phys. Chem. 1967, 71, 2283-9. VARIABLES: PREPARED BY: One temperature: 25°C M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 25°C was reported to be  $0.00297 \text{ mol}(2) \text{dm}^{-3} \text{ sln.}$ 

With the assumption of a solution density of 0.7739 g cm<sup>-3</sup> (density value of pure cyclohexane reported in ref 2), the corresponding mass percent is 0.0069 g(2)/100 g sln and the corresponding mole fraction,  $x_2$ , is 3.2 x  $10^{-4}$  (compiler).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Solubility of (2) in (1) was obtained using the solute isopiestic method described in ref 1. samples were titrated by the Karl Fischer method using a Beckman KF-3 aquameter. The Karl Fisher reagent was standardized alternatively by titrating weighed amounts of sodium tartrate dihydrate or by titrating a 25° 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:

temp. ± 0.1 K

- Christian, S.D.; Affsprung, H.E.; Johnson, J.R.; Worley, J.D. J. Chem. Educ. 1963, 40, 419. 2. Goldman, S. Can. J. Chem. 19
  - 1974, 52, 1668.

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Rebert, C. J.; Hayworth, K. E. Am. Inst. Chem. Engnrs. J. 2. Water; H<sub>2</sub>O; [7732-18-5] 1967, 13, 118-121. VARIABLES: PREPARED BY: C. L. Young Pressure and temperature along one phase-two phase boundary. EXPERIMENTAL VALUES: Smoothed data T/K T/°C P/MPa p/psi g(1)/100 g $x_{C_6H_{12}}$ (soln.) 0.0059 2.7 11.43 1657 593 320 13.06 1894 330 603 340 14.92 2164 613 16.86 2445 623 350 19.21 2785 360 633 643 370 21.83 3165 643.8<sup>a</sup> 22.14 370.6 3210 320 22.06 3199 643 20.07 2910 633 360 2646 623 350 18.25 613 340 16.65 2414 15.23 2209 330 603 593 320 14.17 2054 1942 13.39 583 310 1920 307 13.24 580 1916 577 304 13.21 1925 13.28 302 575 573 300 13.69 1985 568 295 15.88 2303 2540 565 292 17.52 290 18.63 2702 563 1952 603 330 13.46 0.021 9.0 613 340 15.44 2239 2566 623 350 17.70 (cont.)

### AUXILIARY INFORMATION

### METHOD APPARATUS/PROCEDURE:

Samples of mixtures of known composition confined over mercury. Samples 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 ref. (1).

### SOURCE AND PURITY OF MATERIALS:

1. No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$ 

 $\delta p/\text{psi} = \pm 1.$ 

### REFERENCES:

1. Rebert, C. J.; Kay, W. B. Am. Inst. Chem. Engnrs. J. 1959, 5, 285.

### COMPONENTS: ORIGINAL MEASUREMENTS:

2. Water; H<sub>2</sub>O; [7732-18-5]

1. Cyclohexane;  $C_6H_{12}$ ; [110-82-7] Rebert, C. J.; Hayworth, K. E.

Am. Inst. Chem. Engnrs. J.

<u>1967</u>, 13, 118-121.

EXPER	TMENT	PAT. 1	JAT.	UES:

		Smoothed	data		
T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	<sup>ж</sup> С <sub>6</sub> Н <sub>12</sub>
				(soin.)	
633	360	20.61	2989	9.0	0.021
635	362	21.38	3100		
636.5	363.3	21.94	3182		
635 633 _	362 360	22.32 22.45	3236 3255		
632.6 <sup>a</sup>	359.4	22.45	3261		
632	359	22.51	3264		
631	358	22.54	3269		
629	356	22.62	3280		
627	354	22.71	3294		
625	352	22.81	3308		
623	350	22.96	3329		
621	348	23.16	3358		
619	346	23.48	3405	22.2	0.0066
507	235	3.68	533	33.3	0.0966
517 527	245 255	4.36	632 751		
537	265 265	5.18 6.10	885		
547	275	7.12	1032		
557	285	8.25	1196		
567	295	9.57	1388		
573	300	10.30	1494		
578	305	11.07	1605		
583	310	11.96	1734		
588	315	12.87	1866		
593	320	13.79	2000		
598	325	14.96	2169		
603	330	16.13 17.50	2339		
608 613	335 340	19.07	2538 2765		
493	220	3.68	533	60.0	0.0243
503	230	4.47	648	55.5	0.02.0
513	240	5.35	776		
523	250	6.30	914		
533	260	7.45	1081	94.8	0.0796
543	270	8.78	1273		
553	280	10.29	1492		
563	290	12.17	1764		
573	300	14.32	2076		
583 493	310 220	17.79 2.42	2580 351		
503	230	2.88	417		
513	240	3.42	496		
523	250	4.09	593		
533	260	4.86	705		
535	262	5.06	734		
537	264	5.28	765		
539	266	5.54	803		
542.1	268.9	6.25	906		
541	268	6.60	957 976		
540.4 540	267.2 267	6.73 6.76	976 980		
536	263	7.06	1024		
534	261	7.08	1027		
533	260	7.06	1024		
528	255	6.93	1005		
523	250	6.76	980		
E10	245	6.56	951		
516.4 <sup>b</sup>	243.2	6.48	939		
					(cont.)
·	<del></del>				

### ORIGINAL MEASUREMENTS:

1. Cyclohexane;  $C_6H_{12}$ ; [110-82-7] Rebert, C. J.; Hayworth, K. E.

2. Water; H<sub>2</sub>O; [7732-18-5]

Am. Inst. Chem. Engnrs. J.

<u>1967</u>, *13*, 118-121.

EXPERIMENTAL	VALUES:				
		Smoothed	data		
T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	<sup>ж</sup> С <sub>6</sub> Н <sub>12</sub>
	Three ph	ase equilibr	ium locus		
403	130	0.66	95		
413	140	0.86	124		
423	150	1.08	156		•
433	160	1.32	192		
443	170	1.63	237		
453	180	2.01	291		
463	190	2.46	357		
473	200	2.99	433		
483	210	3.58	519		
493	220	4.32	627		
503	230	5.18	751		
508	235	5.64	818		
513	240	6.14	890		
518	245	6.68	968		
523	250	7.28	1055		
528	255	7.92	1148		
528.9	255.7	8.01	1162		
	a Critical	point.			
	b Three-ph	ase point.			

- (1) Cyclohexane;  $C_6H_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Burd, S.D.; Braun, W.G.

Proc. Div. Refining, Am. Petrol. Inst. 1968, 48, 464-76.

### VARIABLES:

PREPARED BY:

Temperature and pressure

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

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

p/psia	p/MPa (compiler)	t/°F	T/K (compiler)	g(2)/100 g sln	x2 (compiler)
25	0.172	202	367.59	0.22	0.0102
50	0.345	241	389.26	0.46	0.0211
100	0.689	284	413.15	0.82	0.0372
150	1.034	312	428.70	1.20	0.0537
200	1.379	333	440.37	1.58	0.0698
250	1.724	350	449.81	1.93	0.0842
300	2.068	364	457.60	2.25	0.0971
350	2.413	377	464.82	2.60	0.1109
400	2.758	388	470.93	3.00	0.1262
24	0.165	200	366.48	0.22	0.0102
59	0.407	250	394.26	0.49	0.0225
127	0.876	300	422.04	1.03	0.0464
250	1.724	350	450.82	1.90	0.0830
450	3.103	400	477.60	3.70	0.1520

### 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, indicating three-phase conditions. Many details are given in the paper.

### SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Company;
  99.5% purity.
- (2) laboratory distilled.

### ESTIMATED ERROR:

soly. ± 0.004 weight fraction of
the (2) present.

### COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] (2) Water; H<sub>2</sub>O; [7732-18-5] Ber. Bunsenges. Phys. Chem. 1970, 74, 682-6. VARIABLES: Pressure and temperature on one phase-two phase boundary. CRIGINAL MEASUREMENTS: Brollos, K.; Peter, K.; Schneider, G. M. Pressure and temperature on one phase-two phase boundary.

### **EXPERIMENTAL VALUES:**

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

T/K	p/bar	<i>*</i> 1	g (1)/100 g soln
379.8	1742	0.100	34.1
369.0	1403		
363.0	1200		
360.1	1000		
351.5	798		
343.5	595		
333.7	395		
329.2	328		
330.0	293		
333.0	271		
334.2	245		
338.0	217		
392.2	1600	0.150	45.2
384.0	1400		
376.5	1202		
369.2	1000		
361.2	800		
351.0	600		
346.5	500		
340.0	394		
338.0	347		
339.0	299		
			(cont.)

### 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:

- Merck sample purity 99.9 mole per cent.
- 2. Twice distilled.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  $\delta P/P = \pm 0.01$ 

(estimated by compiler)

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Cyclohexane; $C_6H_{12}$ ; [110-82-7] Brollos, K.; Peter, K.; Schneider, G. M. (2) Water; $H_2O$ ; [7732-18-5] Ber. Bunsenges. Phys. Chem. 1970, 74, 682-6.

175 1 o a a f	~~~~~~~	~~4	temperature	~~	440	~~~	nh	~h~~~	haundamı
varues or	Diessure	ana	Lemberature	On	CHE	one	Unase-ewo	Duase	Doundarv

T/K	p/bar	<i>x</i> 1	g (1)/100 g soln
340.5	250	0.150	45.2
357.7 403.5	222 1610	0.200	53.9
393.9	1408	0.200	33.3
387.0	1204		
378.7	1002		
369.0 359.5	800 600		
352.2	500		
347.0	416		
343.0	328		
342.0	298		
345.0 355.0	246 223		
412.4	1600	0.298	66.5
404.7	1400		
396.2	1200		
387.1	1004		
375.3 363.8	800 600		
360.4	550		
349.2	398		
346.2	339		
346.5 349.5	237 224		
352.7	214		
414.9	1600	0.400	75.7
406.5	1398		
399.2	1200		
390.1 378.0	995 800		
364.3	600		
355.6	465		
347.6	352 305		
345.0 342.0	295 230		
335.0	195		
421.5	1718	0.500	82.4
419.0	1645		
416.5 408.0	1584 1406		
399.0	1195		
388.9	1004		
376.0	789		
364.0 350.0	600		
350.0 340.1	460 375		
343.0	330		
338.5	250		
330.0	200	0.600	0.5
413.0 405.4	1603 1405	0.600	87.5
395.8	1200		
386.4	1000		
375.3	800		
362.0 345.7	595		
345.7 336.2	395 319		
333.4	290		(cont.)

- (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Brollos, K.; Peter, K.; Schneider, G. M.

Ber. Bunsenges. Phys. Chem. <u>1970</u>, 74, 682-6.

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

T/K	p/bar	$x_1$	g (1)/100 g soln
329.4	261	0.600	87.5
326.5	243		
323.1	220		•
318.5	205		
406.7	1600	0.700	91.6
399.0	1405		
389.1	1200		
380.5	1000		
367.2	800		
351.1	588		
332.5	400		
325.0	342		
314.0	299		
300.5	250		
395.4	1605	0.800	96.9
387.1	1403		
377.6	1200		
367.2	1005		
353.9	800		
337.5	600		
316.5	400		
305.0	295		
295.1	244		
275.2	200		

- (1) Cyclohexane;  $C_6H_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Roddy, J.W.; Coleman, C.F.

Talanta 1968, 15, 1281-6.

### VARIABLES:

One temperature: 25°C

### PREPARED BY:

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 25°C was reported to be  $0.00345 \text{ mol}(2) \text{ dm}^{-3}$  sln corresponding to a mole fraction,  $x_2$ , of  $3.75 \times 10^{-4}$ . 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<sup>-1</sup> (density of cyclohexane reported in ref 1).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A method of gravimetric absorption monitored by tritium tracer was (1) was equilibrated with used. a slight excess of tritiated water by shaking over a period of at least 8 hr in a thermostat. The The phases were allowed to separate for at least 16 hr 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; spectralgrade reagent.
- (2) tritiated water at 5 Ci/mL; New England Nuclear Corp.; diluted to about 1 mCi/mL.

### ESTIMATED ERROR:

soly. better than 1% (type of error
not specified)

### REFERENCES:

1. Goldman, S. Can. J. Chem., 1974, 52, 1968.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7] (2) Water; H <sub>2</sub> O; [7732-18-5]	Plenkina, R.M.; Pryanikova, R.O.; Efremova, G.D.  Zh. Fiz. Khim. 1971, 45, 2389 Deposited doc. 1971, VINITI 3028-71.		
VARIABLES:	PREPARED BY:		
Temperature: 130-250°C	A. Maczynski		

### EXPERIMENTAL VALUES:

### Solubility of water in cyclohexane

t/°C	<sup>x</sup> 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

MALLETAN INCOME OF				
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The solubility of (2) in (1) was determined in sealed glass tubes.	(1) source not specified; CP reagent; crystallized several times; m.p. 6.50°C.			
	(2) distilled.			
	ESTIMATED ERROR:			
	temp. ± 0.5 K			
	REFERENCES:			

- (1) Cyclohexane;  $C_6H_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Glasoe, P.K.; Schultz, S.D.

J. Chem. Eng. Data 1972, 17, 66-8.

### VARIABLES:

PREPARED BY:

Temperature: 15-30°C

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

### Solubility of water in cyclohexane

t/°C ——	mol(2)dm <sup>-3</sup> sln	g(2)/100 g sln (compiler)	10 <sup>4</sup> x <sub>2</sub> (compiler)
15	0.0026 ± 0.0001	0.0060 <sup>a</sup>	2.8
25	0.0032 ± 0.0002	0.0074 <sup>a</sup>	3.5
30	0.0037 ± 0.0002	0.0087 <sup>a</sup>	4.1

acalculated with the assumption of a solution density of 0.7831, 0.7739 and 0.7692 g cm<sup>-3</sup> at respectively 15, 25 and 30°C; these values are the density values of pure cyclohexane at these temperatures (ref 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 using standard 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:

soly.: see above (type of error not specified.

### REFERENCES:

1. Timmermans, J. Physico-chemical constants of pure organic compounds Elsevier, 1950.

### COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Pierotti, R.A.; Liabastre, A.A. (2) Water; H<sub>2</sub>O; [7732-18-5] "Structure and properties of water solutions" U.S. Nat. Tech. Inform. Serv., PB Rep., 1972, No. 21163, 113 pp. VARIABLES: PREPARED BY: Temperature: 278.26-318.36 K M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

### Solubility of cyclohexane in water

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

### 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 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) Fisher Scientific Co.; certified grade; used as received.
- (2) laboratory distilled water.

### ESTIMATED ERROR:

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

- (1) Cyclohexane;  $C_6H_{12}$  [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Leinonen, P.J.; Mackay, D.

Can. J. Chem. Eng. 1973, 51, 230-3.

### VARIABLES:

PREPARED BY:

One temperature: 25°C

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C was reported to be  $56.7 \text{ mg}(1) \text{ dm}^{-3} \text{ sln}$ .

With the assumption of a solution density of 1.00 g cm $^{-3}$ , the corresponding mass percent is 0.00567 g(1)/100 g sln and the corresponding mole fraction,  $x_1$ , is 1.21 x  $10^{-5}$  (compiler).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was equilibrated for at least 12 hrs in a 200 mL Teflon stoppered vessel with gentle shaking. The solution was allowed to settle for 6 hrs and the aqueous phase was tested (Tyndall effect). Both phases were analysed by the gas chromatographic technique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analysed 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:

temp.  $\pm$  0.1 K soly.  $\pm$  1 mg(1)dm<sup>-3</sup> sln

- (1) Cyclohexane;  $C_6H_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Goldman, S.

Can. J. Chem. 1974, 52, 1668-80.

VARIABLES:

PREPARED BY:

Temperature: 10-40°C

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

### Solubility of water in cyclohexane

t/°C	mol(2)dm <sup>-3</sup> sln	g(2)/100 g sln (compiler)	10 <sup>4</sup> x <sub>2</sub> (compiler)
10	0.00147	0.0034 <sup>a</sup>	1.6
15	0.00185	0.0043 <sup>a</sup>	2.0
20	0.00255	0.0059 <sup>a</sup>	2.8
25	0.00301	0.0070 <sup>a</sup>	3.3
30	0.00410	0.0096 <sup>a</sup>	4.5
35	0.00485	0.0114 <sup>a</sup>	5.3
40	0.00552	0.0131 <sup>a</sup>	6.1

<sup>&</sup>lt;sup>a</sup>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 cm<sup>-3</sup> at respectively 10, 15, 20, 25, 30, 35 and 45°C; these values are the density values of pure cyclohexane at these temperatures (ref 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 r.p.m. 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.  $d_{A}^{25} = 0.77390 \pm 0.00002$
- (2) distilled.

### ESTIMATED ERROR:

temp. ± 0.02 K

soly. ± 0.00024 (mean of std. dev.)

### REFERENCES:

1. Timmermans, J. Physico-chemical constants of pure organic compounds Elsevier, 1950.

### COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Mackay, D.; Shiu, W.J.; Wolkoff, A.W. (2) Water; H<sub>2</sub>O; [7732-18-5] "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. 1975, 573, 251-8. VARIABLES: not specified M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The authors reported three different values for the solubility of cyclohexane in water: 55.8, 50.2 and 61.7 mg(1)dm<sup>-3</sup> sln. Using the mean value and assuming a solution density of 1.00 g mL<sup>-1</sup>, the corresponding mass percent, calculated by the compiler, is 0.0056 g(1)/100 g sln and the corresponding mole fraction,  $x_1$ , is  $1.2 \times 10^{-5}$ .

### AUXILIARY INFORMATION

### (1) is 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 is possible to calculate the amount of (1) in the original sample.

METHOD/APPARATUS/PROCEDURE:

### SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

### ESTIMATED ERROR:

soly. ± 10% (compiler)

## COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Mackay, D.; Shiu, W.Y. (2) Water; H<sub>2</sub>O; [7732-18-5] Can. J. Chem. Eng. 1975, 53, 239-41. VARIABLES: PREPARED BY: One temperature: 25°C M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C was reported to be  $0.0575 \text{ g(1)} \, \text{dm}^{-3} \text{ sln}$ .

With the assumption of a solution density of 1.00 g cm<sup>-3</sup>, the corresponding mass percent is 0.00575 g(1)/100 g sln and the corresponding mole fraction,  $x_1$ , is 1.23 x  $10^{-5}$  (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 Model 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:

temp. ± 0.1 K

 $soly. \pm 0.0073 g(1)dm^{-3} sln$ 

- (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S.

Zh. Fiz. Khim. 1976, 50, 1344. Deposited doc. 1976, VINITI 438-76.

### VARIABLES:

One temperature: 20°C

### PREPARED BY:

A. Maczynski

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 20°C was reported to be  $x_1 = 1.5 \times 10^{-5}$ .

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  $x_2 = 4.7 \times 10^{-4}$ .

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 Karl Fischer reagent method.

### SOURCE AND PURITY OF MATERIALS:

- (1) source not specified; pure or analytical reagent grade; purity <99.9%.</p>
- (2) not specified.

ESTIMATED ERROR:

not specified.

- (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Kirchnerova, J.; Cave, G.C.B.

Can. J. Chem. 1976, 54, 3909-16.

### VARIABLES:

One temperature: 25°C

### PREPARED BY:

M.C. Haulait-Pirson

### **EXPERIMENTAL VALUES:**

The solubility of water in cyclohexane at 25°C was reported to be  $0.0030 \text{ mol}(2)/\text{dm}^3 \text{ sln.}$ 

With the assumption of a solution density of  $0.7739 \text{ g cm}^{-3}$  (density value of pure cyclohexane reported in ref 1, the corresponding mass percent is 0.0070 g(2)/100 g sln and the corresponding mole fraction,  $x_2$ , is 3.3 x  $10^{-4}$  (compiler).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The Karl Fischer dead-stop backtitration 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 ther-Trials had shown that the mostat. 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);  $d_A^{25}$  0.7734 ± 0.0001
- (2) distilled and de-ionized

### ESTIMATED ERROR:

temp.  $\pm$  0.1 K soly.  $\pm$  0.0002 mol(2)/dm<sup>3</sup> sln (std. dev. from 5 determinations)

### REFERENCES:

1. Goldman, S. Can. J. Chem. 1974, 52, 1668.

- (1) Cyclohexane;  $C_6H_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.

### VARIABLES:

PREPARED BY:

One temperature: 25°C

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C and at system pressure was reported to be 66.5 mg(l)/kg(2). The corresponding mass percent and mole fraction,  $x_1$ , calculated by the compiler are 0.00665 g(l)/l00 g sln and 1.423 x  $10^{-5}$ .

### 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 insured saturation of the (2) phase in 2 to 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:

temp. ± 1 K

soly.  $\pm$  0.8 mg(1)/kg(2)

### COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub> [110-82-7] (2) Water; H<sub>2</sub>O; [7732-18-5] Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. 1973, 47, 1035.

VARIABLES:

Temperature: 200-250°C Pressure: 2.8-78.5 MPa

PREPARED BY:

A. Maczynski

### EXPERIMENTAL VALUES:

### Solubility of water in cyclohexane

t/°C	p/kg cm <sup>-2</sup>	p/MPa (compiler)	*2	g(2)/100 g sln (compiler)
200	29	2.8	0.156	3.81
	50	4.9	0.091	2.10
	100	9.8	0.052	1.16
	150	14.7	0.046	1.02
	200	19.6	0.043	0.95
1	300	29.4	0.042	0.93
	400	39.2	0.042	0.93
ŀ	500	49.0	0.042	0.93
ļ	600	58.8	0.042	0.93
[	700	68.6	0.042	0.93
	800	78.5	0.041	0.91
225	46.2	4.5	0.230	6.01
	50	4.9	0.209	5.35
	100	9.8	0.128	3.05
	150	14.7	0.100	2.32
i	200	19.6	0.087	2.00
1	300	29.4	0.084	1.92
	400	39.2	0.080	1.83
1	500	49.0	0.076	1.73
	600	58.8	0.072	1.63
l	700	68.6	0.068	1.54
1	800	78.5	0.055	1.23
				(continued)

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The experimental technique was described in ref 1. No details reported in the paper.

### SOURCE AND PURITY OF MATERIALS:

- source not specified, chemical reagent grade; purity not specified; used as received.
- (2) distilled.

### ESTIMATED ERROR:

not specified.

### REFERENCES:

 Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. Gazov. Prom. 1971, 4, 6.

### ORIGINAL MEASUREMENTS:

(2) Water; H<sub>2</sub>O; [7732-18-5]

Sultanov, R.G.; Skripka, V.G. Zh. Fiz. Khim. 1973, 47, 1035.

t/°C	p/kg cm <sup>-2</sup>	p/MPa (compiler)	* <u>2</u>	g(2)/100 g sln (compiler)
250	70 100 150 200 300 400 500 600 700 800	6.9 9.8 14.7 19.6 29.4 39.2 49.0 58.8 68.6 78.5	0.345 0.232 0.182 0.165 0.145 0.131 0.122 0.114 0.106	10.13 6.07 4.55 4.06 3.50 3.13 2.89 2.68 2.47 2.32

## COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Korenman, I.M.; Aref'eva, R.P. (2) Water; H<sub>2</sub>O; [7732-18-5] Patent USSR, 553 524, 1977.04.05 C.A. 87:87654 VARIABLES: One temperature: 20°C PREPARED BY: A. Maczynski

### EXPERIMENTAL VALUES:

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 x 10<sup>-5</sup>. The compiler's calculations assume a solution density of 1.00 g mL<sup>-1</sup>.

### AUXILIARY INFORMATION

### 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.

METHOD/APPARATUS/PROCEDURE:

### SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

### ESTIMATED ERROR:

not specified.

# COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Korenman, I.M.; Aref'eva, R.P. (2) Water; H<sub>2</sub>O; [7732-18-5] Zh. Prikl. Khim. 1978, 51, 957-8. VARIABLES: Temperature: 25°C PREPARED BY: A. Maczynski and Z. Maczynska

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at  $25^{\circ}$ C was reported to be  $0.12 \text{ g(1)} \, \text{dm}^{-3} \text{ sln.}$ 

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

### 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:

soly. ± 0.01 g(1)dm<sup>-3</sup> sln (standard deviation from 6 determinations).

- (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice) 1978, 12, 413-7.

### VARIABLES:

### One temperature: 25°C

### PREPARED BY:

M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at  $25^{\circ}$ C was reported to be 66.5 mg(1)/kg(2).

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

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at Second, the mixture of (1) 25°C. and (2) as above was thermostatted at 70°C and then cooled at 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was mea-A Perkin-Elmer model sured by glc. F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

### SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

### ESTIMATED ERROR:

soly. 1.3 mg(1)/kg(2) (standard
deviation from 7-9 determinations)

### COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Rudakov, E.S.; Lutsyk, A.I. (2) Water; H<sub>2</sub>O; [7732-18-5] Zh. Fiz. Khim. 1979, 53, 1298-1300. VARIABLES: PREPARED BY: One temperature: 25°C M.C. Haulait-Pirson

### EXPERIMENTAL VALUES:

The authors reported the partition coefficient  $\alpha$  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,  $C_{\rm S}$  may be taken as the water solubility and  $C_{\rm g}$  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  $C_{\rm g}=\log p-4.269=-2.28$  expressed in moles per liter. Therefore  $C_{\rm S}=6.56\times 10^{-4}$  moles per liter. With the assumption of a solution density of 1.00 g mL<sup>-1</sup>, the corresponding mass percent is 0.0055 g(1)/100 g sln and the corresponding mole fraction,  $x_1$ , is 1.2 x  $10^{-5}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The equilibrium distribution was attained after shaking for 10 min the 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  $\alpha$  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:

soly. ± 10% (estimated by the compiler)

### REFERENCES:

 Hine, J.; Mooker, P.K. J. Org. Chem. <u>1975</u>, 4, 292.

(1) Cyclohexane;  $C_6H_{12}$ ; [110-82-7]

(2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

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 cyclohexane in water at 23.5°C was reported to be .  $0.0052 \pm 0.0002 \text{ g(1)/100 g sln.}$ 

The corresponding mole fraction,  $x_1$  was calculated by the compiler to be  $1.1 \times 10^{-5}$ .

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. 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) 99.9% purity used without further purification
- (2) distilled

### ESTIMATED ERROR:

temp. ± 1.5°C

soly. 4% (average std. dev.)

- (1) Cyclohexane;  $C_6H_{12}$ ; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Tsonopoulos, C.; Wilson, G.M.

A. I. Ch. E. J. 1983, 29, 990-9.

VARIABLES:

Temperature: 313-482 K

Pressure: 0.03-3.0 MPa

PREPARED BY:

G.T. Hefter

### EXPERIMENTAL VALUES:

The solubility of cyclohexane in water

T/K	p / MPa	104 x1	10 <sup>2</sup> g(1)/100 g sln (compiler)
313.15	0.03151	0.156 <sup>b</sup>	0.728
373.15	0.2723	0.379 <sup>b</sup>	1.77
422.04	_ <i>a</i>	1.03	4.81
423.15	1.0032	1.30	6.07
473.15	2.965	3.92	18.3
482.21	_ a	4.93	23.0

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

(continued)

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

All experimental details are given in an Appendix deposited in a Documentation Centre rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, whilst that of (2) in (1) was measured by Karl Fischer titration.

### SOURCE AND PURITY OF MATERIALS;

- (1) No details given
- (2) No details given

### ESTIMATED ERROR:

soly. ± 5% relative; repeatability of replicate analyses. temp. not stated. press. ± 1%; type of error not stated.

- (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
- (2) Water; H<sub>2</sub>O; [7732-18-5]

(continued)

The solubility of water in cyclohexane

T/K	p <sup>a</sup> /MPa	103 x2	g(2)/100 g sln (compiler)
	<del></del>		•
313.15	0.03151	0.887,0.924,1.13	0.021 <sup>a</sup>
373.15	0.2723	4.35, 5.12	0.10 <sup>a</sup>
423.15	1.0082	20.4,24.0	0.47 <sup>a</sup>
473.15	2.965	79.3	1.81

a Average value.

The three phase critical point was reported to be 529.4 K, 8.025 MPa and  $x_1$  = 1.748 x 10<sup>-3</sup> (0.82 g(1)/100 g sln, compiler).

The authors also report equations fitted to their own and literature data over the range 273-529 K, viz.

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

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

## COMPONENTS: (1) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7] Guseva, A.N.; Parnov, E.I. (2) Deuterium oxide; (heavy water); Radiokhimiya 1963, 5, 507-9. D<sub>2</sub>O; [7789-20-0] VARIABLES: PREPARED BY: Temperature: 71-179.5°C A. Maczynski

### EXPERIMENTAL VALUES:

### Solubility of cyclohexane in deuterium oxide

<i>t</i> /°C	10 <sup>4</sup> x <sub>1</sub>	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
143 168	1.48 3.2	0.0622 0.134

### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined in sealed glass tubes.	(1) not specified. (2) distilled.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

- (1) Cyclohexane;  $C_{6}H_{12}$ ; [110-82-7]
- (2) Deuterium oxide (heavy water); D<sub>2</sub>O; [7789-20-0]

### ORIGINAL MEASUREMENTS:

Backx, P.; Goldman, S.

J. Phys. Chem. 1981, 85, 2975-9.

### VARIABLES:

PREPARED BY:

Temperature: 283-313 K

A. Maczynski

### EXPERIMENTAL VALUES:

### Solubility of deuterium oxide in cyclohexane

<i>T/</i> K	104x2	std. dev.	10 <sup>4</sup> 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<sup>25</sup> 0.77390.
- (2) obtained from the manufacturer; minimum isotopic purity of 99.7 atom % D.

### ESTIMATED ERROR:

Temp. ± 0.01 K Std. dev. of soly calcd from 18-32 determinations reported above.