COMPONENTS:	EVALUATOR:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION:

Data for the solubility of 1,2-dichlorobenzene in water have been reported in several papers. The approximate solubility at 298.15 K was reported by Booth and Everson (1) while, somewhat earlier, Klemenc and Low (2) produced measurements between 293 and 333 K. More recent data have been published only between 276 and 307 K (8-11).

The approximate value provided by Booth and Everson is not given further consideration here. The remaining available data from (2, 8-11) have been correlated relative to absolute temperature using a normal polynomial equation:

$$S_1 (g(1)/kg) = 19.2314 - 1.81140 \times 10^{-1}T$$
$$+ 5.6509 \times 10^{-4}T^2 - 5.77683 \times 10^{-7}T^3 \qquad [1]$$

The significance of this equation is that the curve representing the solubility data passes through a minimum at 283.7 K. This behavior is consistent with the theory discussed by Gill et al. (12) for the solubility of aromatic compounds in water.

Recommended solubility values between 273 and 333 K have been calculated from equation [1] and presented in Table 1. The solubility behavior described by equation [1] is shown also in Figure 1 which contains the reported experimental values for the solubility of 1,2-dichlorobenzene in water.

The solubility of water in 1,2-dichlorobenzene has also been investigated and reported by a number of workers (3-7) in the 298 to 318 K temperature range. In general, these solubility values show some irregularity. While the agreement between the measurements of Jones and Monk (5) and those of Wing and Johnston (7) is reasonable, the deviation is considerable in relation to the measurements of Goldman (4) and of Kirchnerova and Cave (6) at 298.15 K. Identical measured values at 298.15 K were reported from the same department of McGill University by Goldman and by Kirchnerova and Cave.

From the description of the experimental measurements and the reliability if the results reported, it is not reasonable to exclude any of the data points except that quoted by Dreisbach (3) from further analysis. Therefore, all the water in 1,2-dichlorobenzene solubility data except that from Dreisbach were combined and incorporated in a regression equation. However, because of the long equilibration times allowed in Goldman and in Kirchnerova and Cave, their data points were given a weight twice as large as those values provided in Jones and Monk and in Wing and Johnston. The correlation equation is given by:

$$\log_{10}x(2) = 2.23134 - 1448.67/T \qquad [2]$$

In this equation, $x(2)$ is the mole fraction solubility of water in the 1,2-dichlorobenzene-water system and T is the Absolute temperature. The calculated solubility values in the 273 and 333 K range are shown in Figure 2 along with the reported values.

The calculated mole fraction values for the solubility of water in 1,2-dichlorobenzene from equation [2] are given in Table 2 together with the corresponding molarities and g(2)/kg values in the temperature range between 293 and 328 K.

COMPONENTS:	EVALUATOR:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION: (Continued)

Table 1. Solubility of 1,2-Dichlorobenzene in Water.

T/K	$10^4 mol(1)/dm^3$	$10g(1)/kg$	$10^5 x(1)$
273.15	9.64	1.42	1.74
278.15	9.20	1.35	1.66
283.15	9.04	1.33	1.63
288.15	9.13	1.34	1.65
293.15	9.44	1.39	1.70
298.15	9.94	1.47	1.80
303.15	10.6	1.57	1.92
308.15	11.4	1.69	2.07
313.15	12.3	1.82	2.23
318.15	13.2	1.97	2.41
323.15	14.2	2.12	2.60
328.15	15.3	2.28	2.79
333.15	16.2	2.43	2.98

Table 2. Solubility of Water in 1,2-Dichlorobenzene.

T/K	$10^2 mol(2)/dm^3$	$10g(2)/kg$	$10x(2)$
293.15	1.73	2.39	1.95
298.15	2.09	2.90	2.36
303.15	2.50	3.48	2.84
308.15	2.98	4.17	3.39
313.15	3.53	4.96	4.03
318.15	4.16	5.86	4.76
323.15	4.87	6.90	5.60
328.15	5.68	8.08	6.56

COMPONENTS:	EVALUATOR:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION: (Continued)

REFERENCES

1. Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* 1948, *40(8)*, 1491-3.

2. Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas* 1930, *49(4)*, 629-40.

3. Dreisbach, R. R. "Physical Properties of Chemical Compounds," Advances in Chemistry Series No. 15; American Chemical Society: Washington, D.C., 1955; p. 135.

4. Goldman, S., Ph.D. Dissertation, McGill University, Montreal, 1969, p 84.

5. Jones, J. R.; Monk, C. B. *J. Chem. Soc.* 1963, *Part III*, 2633-5.

6. Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* 1976, *54(24)*, 3909-16.

7. Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.

8. Chiou, C. T.; Freed, V. H. "Chemodynamic Studies on Bench Mark Industrial Chemicals"; National Technical Information Service: Springfield, Virginia, 1977; PB-274263.

9. Schwarz, F. P.; Miller, J. *Anal. Chem.* 1980, *52(13)*, 2162-4.

10. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* 1980, *14(10)*, 1227-9.

11. Chiou, C. T.; Schmedding, D. W.; Manes, M. *Environ. Sci. Technol.* 1982, *16(1)*, 4-10.

12. Gill, S. J.; Nichols, N. F.; Wadso, I. *J. Chem. Thermodyn.* 1976, *8(5)*, 445-52.

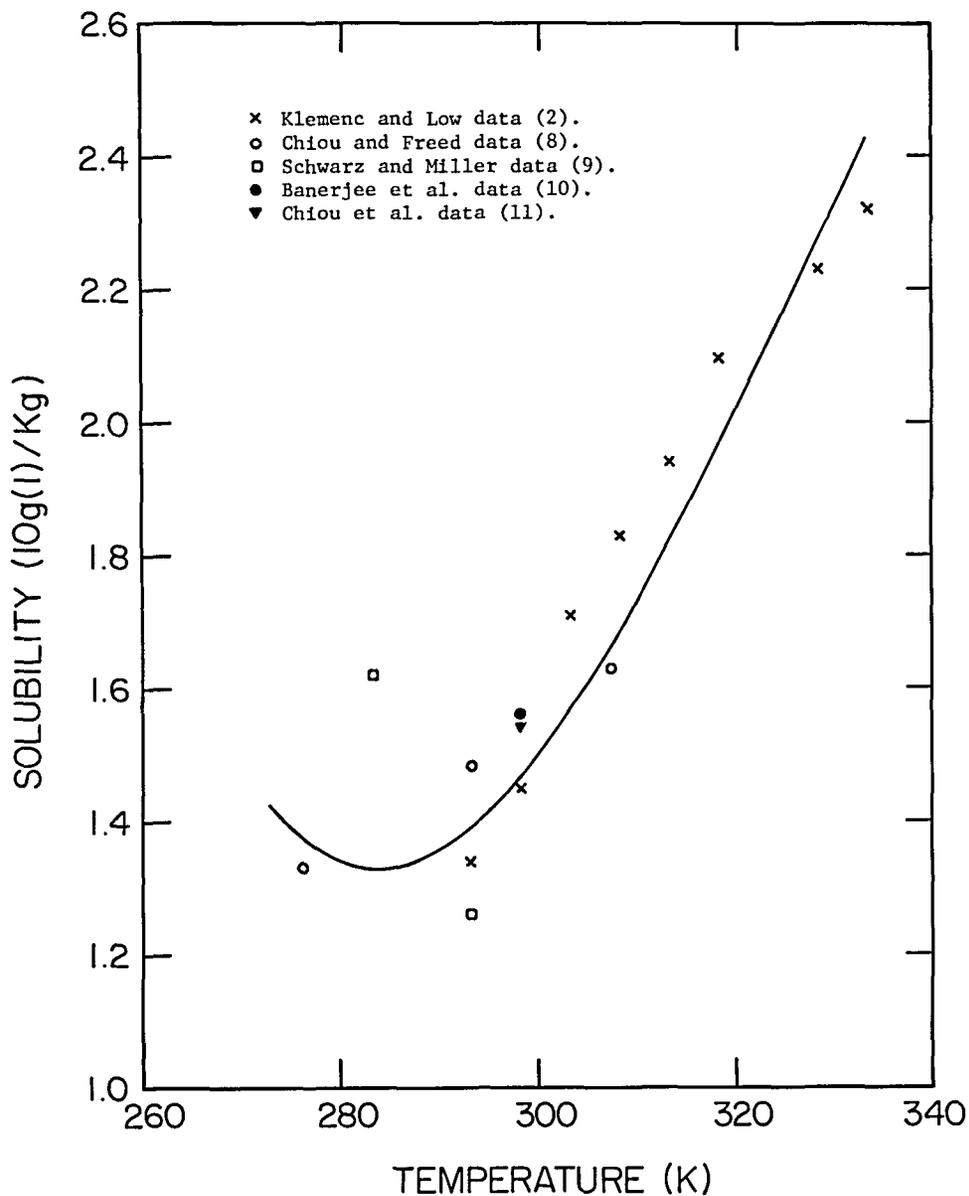| COMPONENTS:	EVALUATOR:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION: (Continued)

Figure 1.   Solubility of 1,2-dichlorobenzene in water versus Absolute
temperature, reported and calculated values.

COMPONENTS:	EVALUATOR:
(1) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	January 1983.

CRITICAL EVALUATION: (Continued)
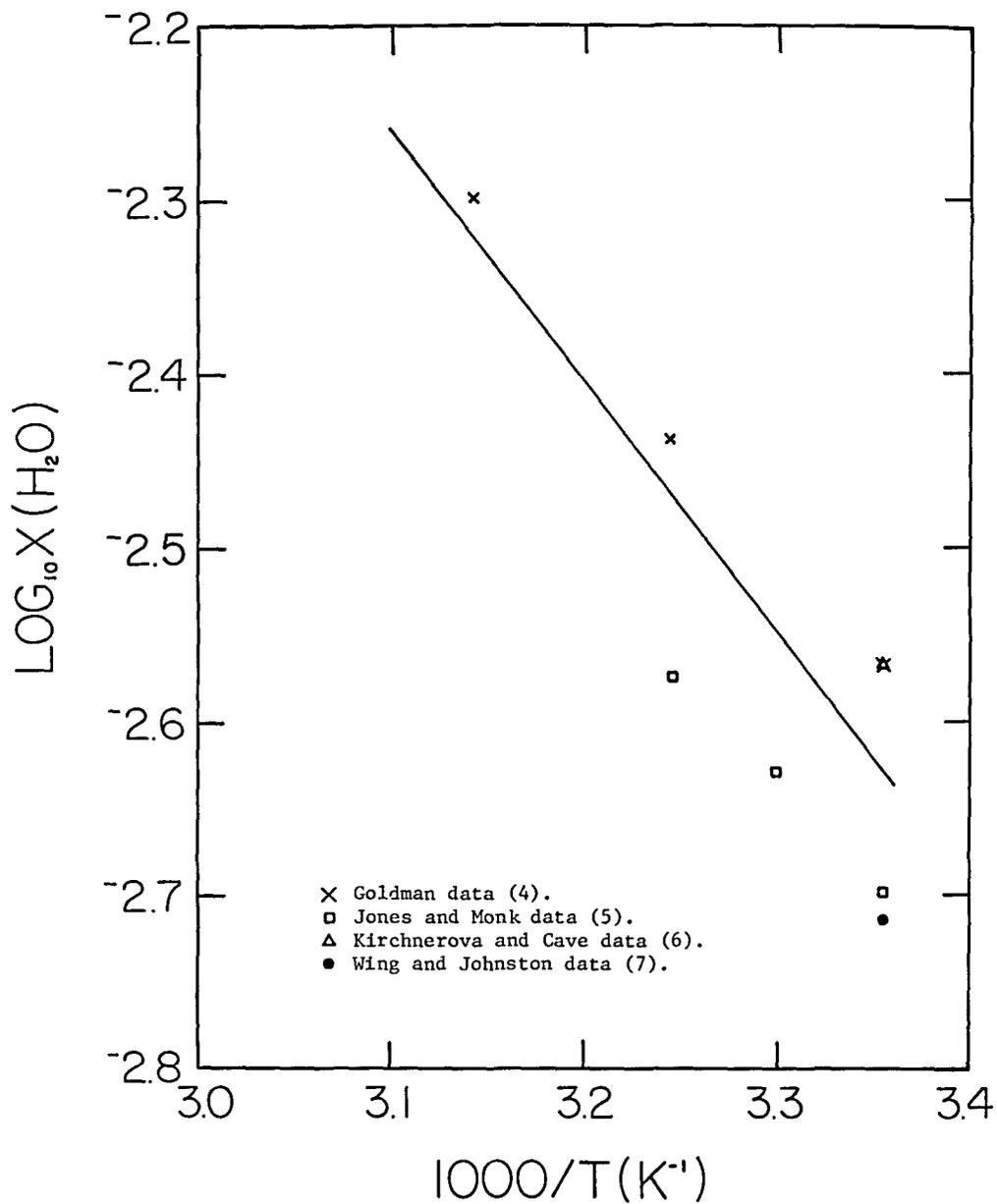
Figure 2.   Logarithm of water mole fraction versus the reciprocal of Absolute temperature for water in 1,2-dichlorobenzene.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas.* 1930, *49(4)*, 629-40.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
20	1.34	0.9114	1.642
25	1.45	0.9862	1.777
30	1.71	1.163	2.096
35	1.83	1.245	2.243
40	1.94	1.319	2.377
45	2.03	1.381	2.488
55	2.23	1.517	2.733
60	2.32	1.578	2.843

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The determination of the solubility was based upon volumetric principles applied to the measurement of excess solute in a calibrated apparatus as described by Rex (1).	$C_6H_4Cl_2$: Kahlbaum reagent, used as received. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±10% (compiler). Temperature: ±1 K (compiler).
	REFERENCES: 1. Rex, A. *Z. Phys. Chem.* 1906, *55*, 355-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Booth, H. S.; Everson, H. E., *Ind. Eng. Chem.* 1948, *40*, 1491-3.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1} ml(1)/dm^3(2)$ [a]	$10 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	< 2	< 1.7	< 3.2

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made with samples contained in a stoppered Goetz tube placed in a constant temperature water bath. Equilibrium was assured through repeated shaking and centrifuging the mixture in the stoppered tube while it was temporarily removed from the water bath. The amount of solute dissolved was determined as the difference between total amount added and amount remaining in excess upon saturation. The determination of the excess amount of solute added has been described by Hanslick (1).	$C_6H_4Cl_2$: Commercial reagent, C. P. grade, used as received. H_2O: Distilled.

| | ESTIMATED ERROR: |
| Solubility: <100% |
| Temperature: ±1 K (compiler). |

| | REFERENCES: |
| 1. Hanslick, R. S., Dissertation, Columbia University, 1935. |

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Dreisbach, R. R. "Physical Properties of Chemical Compounds", Advances in Chemistry Series No. 15; American Chemical Society: Washington, D. C., 1955; p 135.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/kg(2)$ [a]	$mol(1)/kg$ [b]	$10x(1)$ [c]
25	2.1	1.14	1.46

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experimental methods were not described.	H_2O: Distilled. $C_6H_4Cl_2$: Dow Chemical Co., 99.85% pure, purified by distillation before use.
	ESTIMATED ERROR: Solubility: <100% (compiler). Temperature: ±1 K (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10 m l(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	3.09	1.710	1.930

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was equilibrated with 20 ml 1,2-dichlorobenzene by stirring in a flask in a constant temperature water bath for two hours. The concentration of the tritiated water in the organic phase was determined by isotopic dilution. The tritium activities in the tritiated water samples were determined by the acetylene method (1,2). At least four independent experiments were done. The article was based upon work reported in a Ph.D. dissertation (2).	H_2O: Tracerlab Inc., tritiated water, used as received. $C_6H_4Cl_2$: Source not specified, chemical grade, redistilled before use.

ESTIMATED ERROR:
Solubility: ±1.5%.
Temperature: ±0.02 K.

REFERENCES:
1. Wing, J.; Johnston, W. H. *Science* 1955, *121*, 674-5. 2. Wing, J., Ph. D. Dissertation, Purdue University, Lafayette, 1956.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Jones, J. R.; Monk, C. B. *J. Chem. Soc.* <u>1963</u>, *Part III*, 2633-5.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10 ml(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	3.2	1.77	2.00
30	3.75	2.072	2.348
35	4.25	2.344	2.667

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was shaken with 1,2-dichlorobenzene in 1:10 volume ratios for 4 hours in a flask in a water thermostat bath. The water content was determined by tritium assay. The count rates were determined using a typical liquid scintillator solution technique.	H_2O: Tritiated. $C_6H_4Cl_2$: Source not known, laboratory grade, dried over $CaCl_2$ and fractionally distilled before use.

ESTIMATED ERROR:
Solubility: ±5%.
Temperature: ±0.5 K (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Goldman, S., Ph.D. Dissertation, McGill University, Montreal, 1969, p. 84.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^2mol(1)/dm^3$ [b]	$10^3x(1)$ [c]
25.0	4.342	2.41	2.719
35.1	5.783	3.21	3.650
45.06	7.909	4.39	5.028

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium experiments were carried out in a constant temperature water bath using a stirrer. An equilibration period of at least 5 days was allowed. The total water content in the organic phase was determined by a Karl Fischer titration. Each reported water solubility was obtained as an average of at least two independent determinations.	H_2O: Distilled. $C_6H_4Cl_2$: Reagent grade, washed with conc. H_2SO_4 and with 1 M $NaHCO_3$ and then fractionally distilled over silica gel.
	ESTIMATED ERROR: Solubility: ±4%. Temperature: ±0.1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2,-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* *1976*, *54(24)*, 3909-16.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ a	$10^2mol(1)/dm^3$ b	$10^3x(1)$ c
25	4.324	2.40	2.707

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 50 ml 1,2-dichlorobenzene and 6 ml water in a bottle was submerged in a water thermostat bath for 2 days. The concentration of the water in the organic phase was determined by a conventional Karl Fischer dead stop back titration. Determinations were done in triplicate. A detailed description of the complete experimental procedure has been included in a Ph.D. dissertation (1).	H_2O: Distilled and deionized. $C_6H_4Cl_2$: Fisher – B255, washed with cc. H_2SO_4 and K_2SO_3 solution and distilled water. Dried over silica gel and fractionally distilled, purity 99.8%.
	ESTIMATED ERROR: Solubility: ±1%. Temperature: ±0.1 K.
	REFERENCES: 1. Kirchnerova, J., Ph.D. Dissertation, McGill University, Montreal, Quebec, 1974.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Chiou, C. T.; Freed, V. H. "Chemodynamic Studies on Bench Mark Industrial Chemicals"; National Technical Information Service: Springfield, Virginia, 1977; PB-274263.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3(2)$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
3	1.33	0.9046	1.630
20	1.48	1.007	1.817
34	1.62	1.102	1.997

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,2-dichlorobenzene, 5-10 g, was equilibrated with 100 ml distilled water in a bottle for 24 hours at constant temperature. The saturated aqueous phase was removed from the container and analyzed by gas chromatography using a chromatograph equipped with a Ni^{63} EC detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on the determinations and evaluations of experimental procedures have been included in (1).	$C_6H_4Cl_2$: Commercial reagent, used as received. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±10% (compiler). Temperature: ±0.5 K.
	REFERENCES: 1. Chiou, C. T.; Schmedding, D. W. Test. Protoc. Environ. Fate Mov. Toxicants, Proc. Symp., 1980 (Publ. 1981), pp 28-42.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Schwarz, F. P.; Miller, J. *Anal. Chem.* <u>1980</u>, *52(13)*, 2162-4.

VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

Experimentally determined values:

10g(1)/kg

t/°C	Elution Chromatography	UV Absorption
10.0	1.69 ± 0.03	1.56 ± 0.17
20.0	1.28 ± 0.06	1.24 ± 0.04

Values derived from average measured solubilities:

t/°C	10g(1)/kg [a]	10^3mol(1)/kg [b]	$10^5 x(1)$ [c]
10.0	1.62 ± 0.07	1.102 ± 0.048	1.986 ± 0.086
20.0	1.26 ± 0.02	0.8571± 0.0136	1.544 ± 0.025

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Both elution chromatography and UV absorption methods were used to determine the aqueous solubilities. The agreement was within an experimental error of 4% between the two methods. The average deviations were determined from several measurements made on different samples. The analytical procedures for determining organic liquid solubilities in water based on liquid phase elution chromatography has been described in (1).	$C_6H_4Cl_2$: Commercial, 98 wt. %. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±4%. Temperature: ±0.5 K.
	REFERENCES: 1. Schwarz, F. P. *Anal. Chem.* <u>1980</u>, *52(1)*, 10-15.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2–dichlorobenzene; $C_6H_4Cl_2$: [95-50-1] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environm. Sci. Techn.* <u>1980</u>, *14(10)*, 1227-9.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25	1.5583	1.060	1.9156

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,2–dichlorobenzene was added to water in a stainless steel centrifuge tube which was then sealed. The equilibrium was established by allowing the sample to stand, with intermittent shaking, for a week at constant temperature. The mixture was then centrifuged and aliquots of the solution were removed either by a pipet or syringe for analysis. Liquid scintillation counting with ^{14}C-labelled solute was employed in the solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.	$C_6H_4Cl_2$: New England Nuclear, used as received. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±0.9% S.D. Temperature: ±0.3 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Chiou, C. T.; Schmedding, D. W.; Manes, M. *Environ. Sci. Technol.* <u>1982</u>, *16(1)*, 4-10.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25	1.5392	1.047	1.8921

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,2-dichlorobenzene was equili-brated with water in screwcapped bottles in a reciprocal shaker for 24 hours. After two days settling, samples were taken from the solution for analysis by gas chromato-graphy. The chromatograph was equipped with a Ni^{63} EC detector. Analyses were continued until a constant concentration was observed.	$C_6H_4Cl_2$: Not specified. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±5% (compiler). Temperature: ±0.5 K.
	REFERENCES: