COMPONENTS:	EVALUATOR:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION:

Seven experimental determinations have been published on the solubility of 1,3-dichlorobenzene in water in various temperature intervals (1-7), see Figure 1. Some rather serious discrepancies between the various solubility measurements are evident in the figure. The discrepancy between the two determinations (3) and (6) is about 47 percent at ambient temperature. The solubility data of Klemenc and Low (1) cover the temperature range between 293 and 333 K, while the measurements of Vesala (2,3) fall in the temperature range between 283 and 308 K. The remaining measurements reported (4-7) fall in the room temperature range.

The solubility measurements of Vesala (2,3) have been taken as most reliable and, therefore, these values were heavily weighed in the correlation of solubility versus Absolute temperature by means of a normal, three degree polynomial equation:

$$S_1(g(1)/kg) = 27.6827 - 2.61597 \times 10^{-1} T + 8.19706 \times 10^{-4} T^2 - 8.4698 \times 10^{-7} T^3 \qquad [1]$$

The significance of this equation representing the solubility data is that the curve passes through a minimum at 298.2 K. This observation is consistent with the theory discussed by Gill et al. (8) for the solubility of aromatic compounds in water.

The errors in the recommended solubility values given below could be as large as ± 10 percent, particularly at the higher temperatures. Recommended solubility values calculated from equation [1] together with corresponding molarity and mole fraction values are listed in Table 1. Also, the solubility values calculated from equation [1] are shown in Figure 1 as a solid line along with the measured values.

Table 1. Solubility of 1,3-Dichlorobenzene in Water.

T/K	10^4mol(1)/dm^3	10g(1)/kg	$10^5x(1)$
283.15	7.01	1.03	1.26
288.15	6.79	0.999	1.22
293.15	6.86	1.01	1.24
298.15	7.19	1.06	1.30
303.15	7.73	1.14	1.40
308.15	8.43	1.25	1.53
313.15	9.24	1.37	1.68
318.15	10.14	1.51	1.84
323.15	11.07	1.65	2.02
328.15	11.98	1.79	2.19
333.15	12.84	1.92	2.35

The recommended molar concentrations and mole fractions have been calculated from the g(1)/kg and the densities of the two components at the equilibrium temperatures indicated.

COMPONENTS:	EVALUATOR:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)

REFERENCES

1. Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas* 1930, *49(4)*, 629-40.
2. Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.
3. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.
4. Chiou, C. T.; Schmedding, D. W.; Maines, M. *Environ. Sci. Technol.* 1982, *16(1)*, 4-10.
5. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* 1980, *14(10)*, 1227-9.
6. Schwarz, F. P. *Anal. Chem.* 1980, *52(1)*, 10-15.
7. Schwarz, F. P., Miller, J. *Anal. Chem.* 1980, *52(13)*, 2162-4.
8. Gill, S. J.; Nichols, N. F.; Wadso, I. *J. Chem. Thermodyn.* 1976, *8(5)*, 445-52.

COMPONENTS:	EVALUATOR:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)

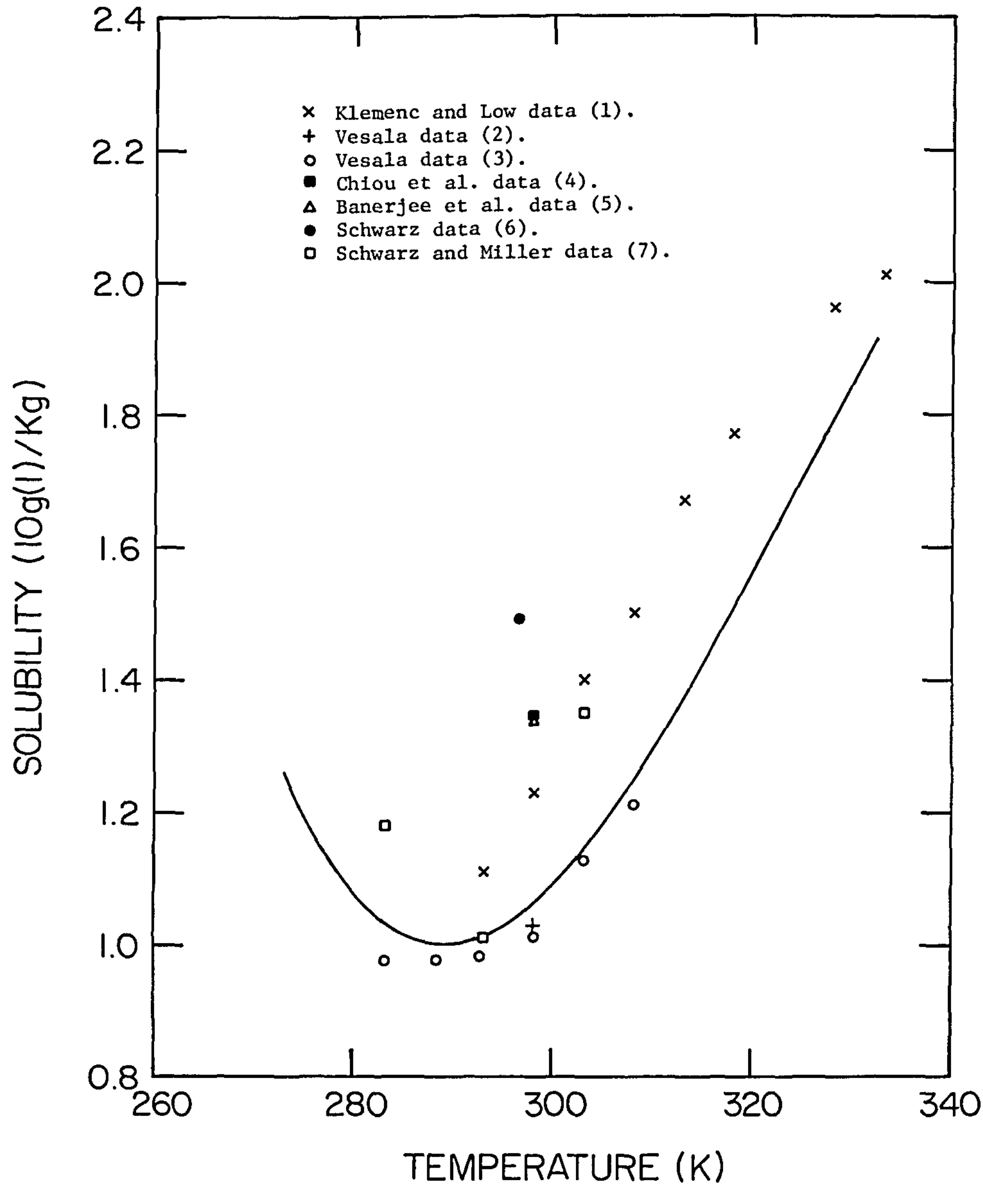

Figure 1. Solubility of 1,3-dichlorobenzene in water versus Absolute temperature, reported and calculated values.

COMPONENTS:

(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

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]	10^3mol(1)/kg [b]	$10^5x(1)$ [c]
20	1.11	0.7550	1.360
25	1.23	0.8366	1.507
30	1.40	0.9522	1.716
35	1.50	1.020	1.838
40	1.67	1.136	2.047
45	1.77	1.204	2.169
55	1.96	1.333	2.402
60	2.01	1.367	2.463

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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).

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: Kahlbaum reagent, purified by the method of Friedel and Crafts before use.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±10% (compiler).

Temperature: ±1 K (compiler).

REFERENCES:

1. Rex, A. *Z. Phys. Chem.* 1906, *55(A)*, 355-70.

COMPONENTS:

(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.

VARIABLES:

Temperature

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10g(1)/kg [a]	10^4mol(1)/kg(2) [b]	$10^5x(1)$ [a]
10.0	0.97632	6.642 ± 0.088	1.1966
15.2	0.97764	6.651 ± 0.091	1.1982
19.6	0.98323	6.689 ± 0.096	1.2051
25.1	1.0126	6.889 ± 0.079	1.2411
30.0	1.1274	7.670 ± 0.061	1.3818
35.0	1.2113	8.241 ± 0.159	1.4847

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The 1,3-dichlorobenzene was mixed with water in a sealed flask (1) with the aid of a magnetic stirrer for 48 hours in a water bath at constant temperature. After the solution was filtered through a glass-wool plug, the solute was extracted with 2,2,4-trimethylpentene. The optical density of each sample was determined spectrophotometrically (2). Mean and standard deviations were calculated from three measurements.

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: Fluka AG, puriss, >99% GLC, used as received.

H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:

Solubility: ±1.93%.

Temperature: ±0.05 K.

REFERENCES:

1. Franks, F.; Gent, M.; Johnson, H. H. *J. Chem. Soc.* 1963, *Part III,* 2716-23.
2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

COMPONENTS:

(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.

VARIABLES:

One temperature

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10g(1)/kg [a]	10^4mol(1)/kg(2) [b]	$10^5x(1)$ [a]
25	1.029	7.00	1.261

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium was established between the water and the 1,3-dichlorobenzene in a sealed flask (1) with the aid of a magnetic stirrer during 48 hours under isothermal conditions. After the sample was filtered through a glass-wool plug, the 1,3-dichlorobenzene was extracted with 2,2,4-trimethylpentene. Sample optical densities were determined spectrophotometrically (2). Five parallel determinations were done.

The reported work was based upon a Ph.D. dissertation (3).

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: Commercial reagent of analytical grade distilled through a column resulting in a more than 99% pure sample.

H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:

Solubility: ±1.0%.

Temperature: ±0.05 K.

REFERENCES:

1. Franks, F.; Gent, M.; Johnson, H. H. *J. Chem. Soc.* 1963, *Part III*, 2716-23.
2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.
3. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.

COMPONENTS:

(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schwarz, F. P. *Anal. Chem.* 1980, *52(1)*, 10-15.

VARIABLES:

One temperature

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10g(1)/kg [a]	10^3mol(1)/kg [b]	$10^5x(1)$ [c]
23.5	1.49 ± 0.11	1.014	1.826
23.5	1.44 ± 0.03	0.9796	1.765

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined by using an elution chromatography analytical technique. The procedure involved the use of an inert solid packing coated with a known amount of solute in a transparent tube. Water was forced through the packed tube to remove amounts of solute. The solubility was calculated from the length of the solute depleted zone (as observed from the color difference between the depleted packing and that in the remaining portion of the tube) and the volume of water passed through the tube. Chemisorb P was used as the inert solid packing.

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: Commercial, 98 wt %.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±7% S.D.

Temperature: ±1.5 K.

REFERENCES:

COMPONENTS:

(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

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

VARIABLES:

Temperature

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

Experimentally determined values:

	10g(1)/kg	
t/°C	Elution Chromatography	UV Absorption
10.0	1.16 ± 0.06	1.20 ± 0.06
20.0	0.89 ± 0.04	1.13 ± 0.05
30.0	1.39 ± 0.07	1.32 ± 0.05

Values derived from average measured solubilities:

t/°C	10g(1)/kg [a]	10^4mol(1)/kg [b]	$10^5 x(1)$ [c]
10.0	1.18 ± 0.02	8.027 ± 0.136	1.446 ± 0.025
20.0	1.01 ± 0.12	6.870 ± 0.816	1.238 ± 0.180
30.0	1.35 ± 0.03	9.183 ± 0.204	1.655 ± 0.037

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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).

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: Commercial, 98 wt. %.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±4%.

Temperature: ±0.5 K.

REFERENCES:

1. Schwarz, F. P. *Anal. Chem.* 1980, *52(1)*, 10-15.

COMPONENTS:

(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

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

VARIABLES:

One temperature

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	1.335	9.08	1.641

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of 1,3-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.

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: New England Nuclear, used as received.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±1.1% S.D.

Temperature: ±0.3 K.

REFERENCES:

COMPONENTS:

(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

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

VARIABLES:

One temperature

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25	1.341	9.12	1.648

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of 1,3-dichlorobenzene was equilibrated 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 chromatography. The chromatograph was equipped with a Ni^{63} EC detector. Analyses were continued until a constant concentration was observed.

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: Not specified.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±5% (compiler).

Temperature: ±0.5 K.

REFERENCES: