COMPONENTS:	EVALUATOR:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION:

Thirteen experimental determinations of the solubility of chlorobenzene in water between 278 and 363 K have been reported in the literature (1-10,23-25), see Figure 1. The solubility at higher temperatures, between 513 and 533 K, have been reported also by Vorozhtsov and Kobelev (11) in graphical form only without further details concerning the source of the original measurements.

The solubility of water in chlorobenzene has been reported in eleven published works (5,9,12-20) in the temperature range between 288 and 322 K, see Figure 2.

Some of the more recent data for the solubility of chlorobenzene in water is that of Nelson and Smit (8) in the temperature range between 278 and 318 K. However, despite equilibrium periods of 24 hours (which might not have been long enough), the measured solubilities are substantially lower than those found by earlier investigators. It is not possible to establish any shortcomings of the experimental procedures from the very brief description. No information was provided on the source and purity of materials used. Also, it was not indicated whether or not a water stripper had been employed for the analysis of the very dilute aqueous solutions by gas chromatography, or whether or not an internal standard had been used for the calibration of the gas chromatograph which employed a flame ionization detector. However, the authors agreed to re-examine their raw data in order to verify the reported values (21). Consequently, for the present evaluation, their results have not been considered for inclusion in the selected solubility values.

The reported solubilities of Othmer et al. (9) and those of Newman et al (23) are too high in relation to the other reported solubility data. Consequently, these values have not been included in the correlation procedure. The approximate value given by Booth and Everson (3) has been excluded also from further consideration. The solubility data at high temperatures by Vorozhtsov and Kobelev (11) could not be correlated with the other data given. These remaining data given in (1,2,4-7,10,24,25) were correlated with Absolute temperature using polynomial equations of various degrees. The equation given below represents the solubility of chlorobenzene in water between 283 and 363 K within an estimated 10 percent. Equal weight was given to each of the data points in the regression procedure for the following equation:

$$S_1(g(1)/kg) = 11.3351 - 3.0290 \times 10^{-2}\, T - 1.8716 \times 10^{-4}\, T^2 + 0.559466 \times 10^{-6}\, T^3 \quad [1]$$

The significance of this equation is that the curve representing the solubility data passes through a minimum at 286.1 K. This behavior is consistent with the theory discussed by Gill et al. (27) for the solubility of aromatic compounds in water.

Recommended solubility values between 283 and 363 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 chlorobenzene in water.

The solubility of water in chlorobenzene has also been investigated and reported by a number of workers (9,13,17,18,19,20,26) in the 298 to 318 K temperature range. In general, these solubility values show some irregularity, but those showing reasonable agreement can be correlated with respect to Absolute temperature. The reported solubilities of Zielinski (20) and of Othmer et al. (9) are too high while those of Jones and Monk (17) are too low. Consequently, these data are not considered further. Also, the solubility expressed as a distribution coefficient by an equation only (26) cannot be included in the correlation. The good agreement of the values at 298.15 K reported in (13,18,19) are heavily weighed in the correlation. The remaining data were all assigned equal weight to produce the following equation:

$$\log_{10} x(2) = 2.99105 - 1668.56/T \quad [2]$$

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

COMPONENTS:	EVALUATOR:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION: (Continued)

The calculated mole fraction values for the solubility of water in chlorobenzene from equation [2] are given in Table 2 together with the corresponding molarities and g(2)/kg values in the temperature range between 283 and 333 K.

The azeotrope temperature (363.35 K) and composition (284 g(2)/kg) at 1.0133 x 10^5 Pa pressure were also reported (22).

Table 1. Solubility of Chlorobenzene in Water.

T/K	10^3mol(1)/dm^3	10g(1)/kg	10^5x(1)
283.15	4.03	4.54	7.27
288.15	4.02	4.52	7.24
293.15	4.13	4.66	7.46
298.15	4.38	4.95	7.92
303.15	4.77	5.39	8.63
308.15	5.30	6.00	9.60
313.15	5.97	6.77	10.84
318.15	6.78	7.71	12.34
323.15	7.74	8.82	14.13
328.15	8.85	10.11	16.20
333.15	10.12	11.58	18.56
338.15	11.53	13.24	21.22
343.15	13.11	15.09	24.18
348.15	14.84	17.13	27.46
353.15	16.73	19.37	31.06
363.15	20.98	24.47	39.24

Table 2. Solubility of Water in Chlorobenzene;

T/K	10^2mol(2)/dm^3	10g(2)/kg	10^3x(2)
283.15	1.24	2.01	1.25
288.15	1.57	2.54	1.59
293.15	1.96	3.19	1.99
298.15	2.43	3.98	2.48
303.15	2.99	4.92	3.07
308.15	3.66	6.05	3.77
313.15	4.44	7.39	4.60
318.15	5.36	8.97	5.58
323.15	6.43	10.82	6.72
328.15	7.67	12.99	8.06
333.15	9.10	15.50	9.61

COMPONENTS:	EVALUATOR:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION: (Continued)

REFERENCES

1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.
2. Aquan-Yuen, M.; Mackay, D.; Shiu, W. Y. *J. Chem. Eng. Data* 1979, *24(1)*, 30-4.
3. Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* 1948, *40(8)*, 1491-3.
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10. Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.
11. Vorozhtsov, N. N.; Kobelev, V. A. *Zh. Obs. Khim.* 1938, *8(12)*, 1106-19.
12. Bell, R. P. *J. Chem. Soc.* 1932, *Part II*, 2905-11.
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19. Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.
20. Zielinski, A. Z. *Chem. Stosowana* 1959, *3*, 377-84.
21. Nelson, H. D., Personal Communication, 1979.
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COMPONENTS:	EVALUATOR:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION: (Continued)

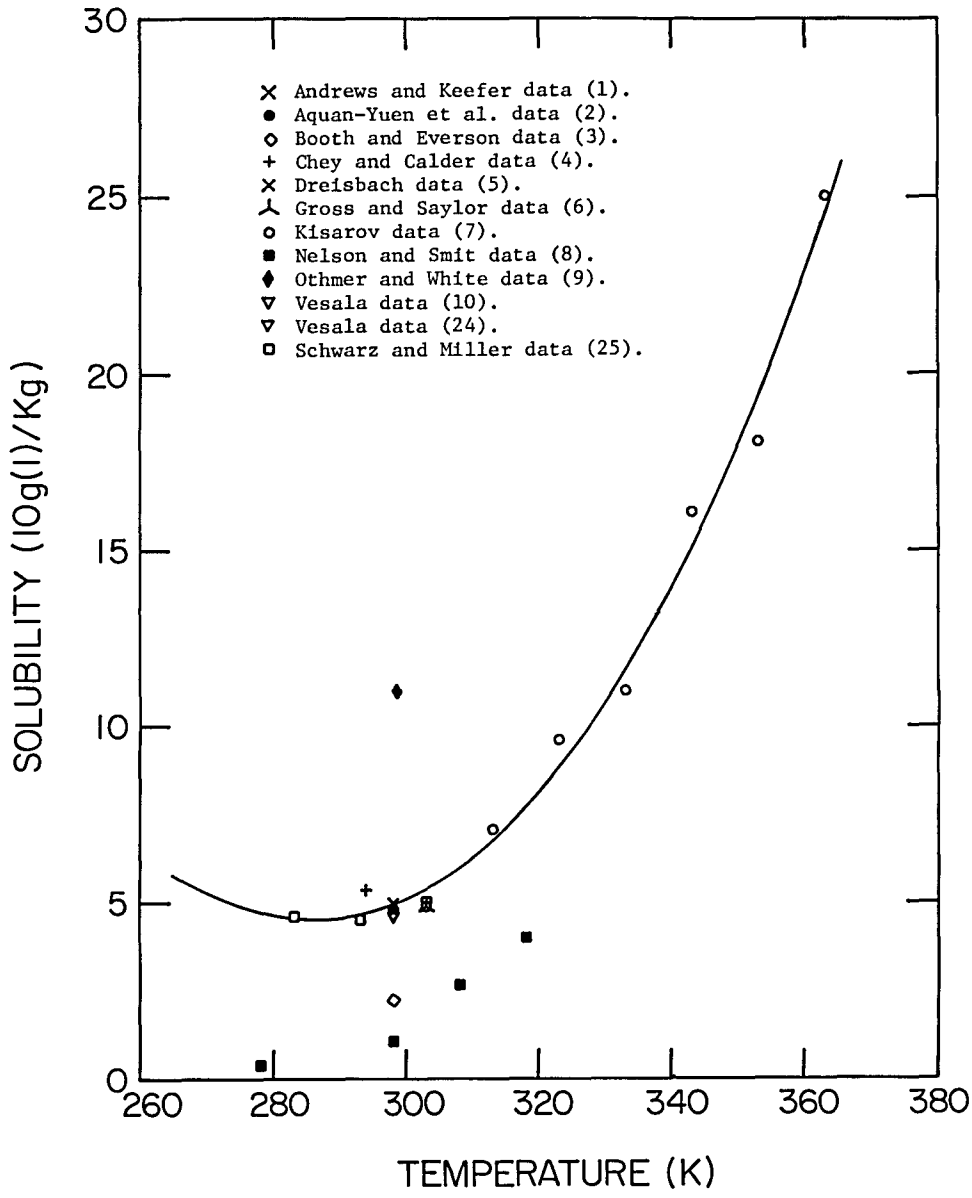

Figure 1. Solubility of chlorobenzene in water versus Absolute temperature, reported and calculated values.

COMPONENTS:	EVALUATOR:
(1) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Chlorobenzene; C_6H_5Cl; [108-90-7]	May 1979.

CRITICAL EVALUATION: (Continued)

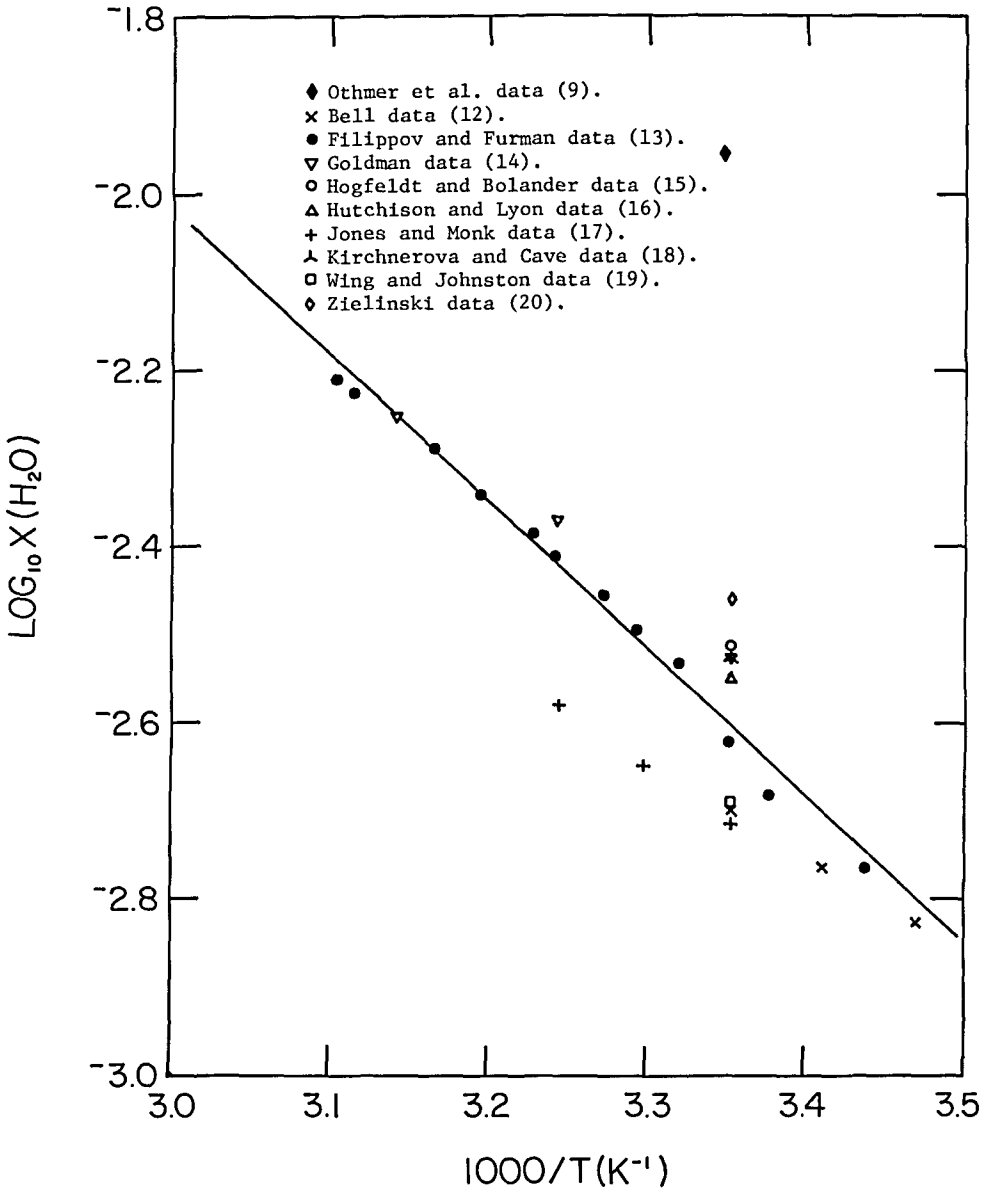

Figure 2. Logarithm of mole fraction solubility of water in chlorobenzene versus reciprocal of Absolute temperature, reported and calculated values.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* 1931, *53(10)*, 1744-51.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
30	4.88	4.333	7.810

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of chlorobenzene in 500 g water was shaken for 12 hours in a thermostat bath. Samples were then withdrawn and read against water as a reference using an interferometer made by Zeiss (1).

A detailed description of the complete procedure has been described in a Ph.D. dissertation (2).

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Eastman Kodak Co., was purified by fractional distillation before use.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±1.0%.

Temperature: ±0.02 K.

REFERENCES:

1. Gross, P. M. *J. Am. Chem. Soc.* 1929, *51(8)*. 2362-6.

2. Saylor, J. H., Ph.D. Thesis, Duke University, Durham, 1930.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Bell, R. P. *J. Chem. Soc.* 1932, Part II, 2905-11.
VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
15	2.64	1.471	1.488
20	3.05	1.691	1.719
25	3.54	1.953	1.995

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Mixtures of solute and solvent in about 1 to 5 ratios were rotated in a thermostat bath for 12 hours. After equilibrium was attained, samples were withdrawn and filtered through cotton-wool. The determination of the water content was based upon the reaction of water with α-naphthoxydichlorophosphine. The evolved HCl was absorbed in water and titrated with standard NaOH solution (1). From 2-4 successive determinations were made with the solvent.

SOURCE AND PURITY OF MATERIALS:

H_2O: Distilled (compiler).

C_6H_5Cl: Merck reagent, analytical grade, redistilled before use.

ESTIMATED ERROR:

Solubility: ±1.6%.

Temperature: ±0.02 K.

REFERENCES:

1. Bell, R. P. *J. Chem. Soc.* 1932, Part II, 2903-5.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Vorozhtsov, N. N.; Kobelev, V. A. *Zh. Obs. Khim.* 1938, *8(12)*, 1106-19.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10^{-1}g(1)/kg [a]	10mol(1)/kg [b]	$10^3 x(1)$ [c]
240	5.8	5.15	9.76
250	6.2	5.51	10.5
260	6.8	6.04	11.5

a. Values obtained from graph plot (Fig. 4).
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Not specified.	Not specified.
	ESTIMATED ERROR: Solubility: ±10% (compiler). Temperature: ±1 K (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Othmer, D. F.; White, R. E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33(12)*, 1513.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	g(1)/kg	10^3mol(1)/kg	10^4x(1)
25.5	1.1	9.77	1.76

t/°C	g(2)/kg	10^2mol(2)/kg	10^2x(2)
25.5	1.8	9.99	1.11

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Measurements were made using about 15 ml water in a 125 ml Erlenmeyer flask (1). The solute was added to the water from a buret and the flask was agitated until the solution became turbid. The amounts of reagent added were converted from volume to mass using the known densities of the pure components.

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Source not specified. Purified until it distilled within 1 or 2°C range.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±10% (compiler).

Temperature: ±0.5 K.

REFERENCES:

1. Othmer, D. F.; White, R. E.; Trueger, E. *Ind. Eng. Chem.* 1941, *33(10)*, 1240-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene: C_6H_5Cl; [108-90-7]	Hutchison, C. A.; Lyon, A. M. Columbia University Report A-745, July 1, 1943.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^3 x(1)$ [c]
25	4.504	2.50	2.807

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Mixtures of 1 to 15 volume ratios of solute to solvent were introduced into an equilibration flask and placed in a water thermostat bath. The assembly was shaken mechanically for about 90 minutes at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration. The determinations were done in triplicate. The experimental procedure was taken from a secondary source (1). The original report is no longer available.

SOURCE AND PURITY OF MATERIALS:

H_2O: Distilled.

C_6H_5Cl: Source is not known, purified and dried before use.

ESTIMATED ERROR:

Solubility: ±1%.

Temperature: ±0.05 K.

REFERENCES:

1. Eidinoff, M. L. In "Production of Heavy Water", National Nuclear Energy Series Division III-Vol. 4F, Murphy, G. M., Urey, H. C., Kirshenbaum, I., Eds.; McGraw-Hill: New York, 1955; Part II, Chapter 7, pp 129-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* 1948, *40(8)*, 1491-3.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10ml(1)/dm^3(2)$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25.0	< 2	< 2.0	< 3.6

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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).

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Commercial reagent, C.P. grade, used as received.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: <100%.

Temperature: ±1 K (compiler).

REFERENCES:

1. Hanslick, R. S., Ph.D. Dissertation, Columbia University, New York, 1935.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Newman, M.; Hayworth, C. B.; Treybal, R. E. *Ind. Eng. Chem.* 1949, *41(9)*, 2039-43.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	g(1)/kg [a]	10^2mol(1)/kg [b]	10^4x(1) [c]
25	4.0	3.55	6.42

t/°C	10g(1)/kg [d]	10^3mol(1)/kg [d]	10^5x(1) [d]
25	4.0	3.55	6.40

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.
d. Calculated for 0.1x reported value by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium between the solute and solvent was established in a constant temperature bath with sufficient agitation. The composition analysis was by standard procedures (1) with specific gravity as the basis of analysis.

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Not specified.

H_2O: Not specified.

ESTIMATED ERROR:

Solubility: Too large by a factor of 10 (compiler).

Temperature: ±0.3 K (compiler).

REFERENCES:

1. Smith, J. C. *Ind. Eng. Chem.* 1942, *34(2)*, 234-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(9)*, 3113-6.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ a	$10^3 mol(1)/dm^3$ b	$10^5 x(1)$ c
25.0	5.0	4.44	8.03

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water was saturated with chlorobenzene in a glass stoppered Erlenmeyer flask by rotating the flask in a constant temperature bath for 20 hours. The saturated solution was extracted with n-hexane for analysis. The optical density of the extract was measured against a n-hexane standard using a Beckman spectrophotometer (1).

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Eastman Kodak Co., commercial reagent, b.p. 131.9-132°C, fractionated before use.

H_2O: Not specified.

ESTIMATED ERROR:

Solubility: ±10% (compiler).

Temperature: ±0.1 K (compiler).

REFERENCES:

1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1949, *71(11)*, 3644-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Filippov, T. S.; Furman, A. A. *Zh. Prikl. Khim.* 1952, *25*, 895-7.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10g(1)/kg [a]	10^2mol(1)/kg [b]	10^3x(1) [c]
17.7	2.75	1.526	1.716
22.9	3.33	1.848	2.077
25.2	3.82	2.120	2.382
28.0	4.70	2.609	2.929
30.4	5.12	2.842	3.190
32.4	5.60	3.108	3.489
35.3	6.21	3.447	3.867
36.6	6.60	3.663	4.109
39.8	7.31	4.058	4.550
42.7	8.25	4.579	5.132
47.9	9.55	5.301	5.937
49.0	9.90	5.495	6.153

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Measured amounts of water and chlorobenzene were introduced into a tared ampoule which was then sealed. The ampoule was constantly shaken in a thermostat at a series of regulated temperatures until it appeared cloudy. Variations in temperature for clouding and clearing conditions were not more than 0.2-0.3°C. This procedure for solubility measurements has been referred to as the cloud point method by Alexejew (1).

SOURCE AND PURITY OF MATERIALS:

H_2O: Double distilled.

C_6H_5Cl: Source not known, distilled three times over freshly calcined calcium oxide.

ESTIMATED ERROR:

Solubility: ±5% (compiler).

Temperature: ±0.1 K (compiler).

REFERENCES:

1. Alexejew, Wladimir *Ann. d. Phys. u. Chem.* 1886, *28*, 305-38.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenezene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Dreisbach, R. R. "Physical Properties of Chemical Compounds", Advances in Chemistry Series No. 15; American Chemical Society: Washington, D. C., 1955; p 134.
VARIABLES: One 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]
25	5.0	4.44	8.00

t/°C	$10^{-1} g(2)/kg(1)$ [a]	$mol(2)/kg$ [b]	$10x(2)$ [c]
25	4.4	2.34	2.16

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No details are available.	C_6H_5Cl: Dow Chemical Co., 99.98% pure, purified by distillation before use. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: (1) in (2) ±10% (compiler). (2) in (1) <100% (compiler). Temperature: ±1 K (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene: C_6H_5Cl; [108-90-7]	Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10ml(1)/dm^3$ a	$10^2 mol(1)/dm^3$ b	$10^3 x(1)$ c
25.0	3.60	1.992	2.035

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Tritiated water was equilibrated with 20 ml chlorobenzene through 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. For the tritiated water samples, the tritium activities were determined by the acetylene method (1,2). At least four independent determinations were made.

The article was based upon work reported in a Ph.D. dissertation (2).

SOURCE AND PURITY OF MATERIALS:

H_2O: Tracerlab Inc., tritiated water, used as received.

C_6H_5Cl: Source not specified, chemical grade, redistilled before use.

ESTIMATED ERROR:

Solubility: ±2.8%.

Temperature: ±0.02 K.

REFERENCES:

1. Wing, J.; Johnston, W. H. *Science* 1955, *121*, 674-6.

2. Wing, J., Ph.D. Dissertation, Purdue University, Lafayette, 1956.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Zieleinski, A. Z. *Chem. Stosowana* 1959, *3*, 377-84.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [b]
25	6.1	3.39	3.45

a. Reported.
b. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Not specified.	Not specified.
	ESTIMATED ERROR: Solubility: ±10% (compiler). Temperature: ±1 K (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Kisarov, V. M. *Zh. Prikl. Khim.* 1962, *35*(10), 2347-9.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(l)/kg$ [a]	$10^3 mol(l)/kg$ [b]	$10^4 x(l)$ [c]
30	4.90	4.353	0.7846
40	7.05	6.263	1.129
50	9.60	8.529	1.538
60	11.00	9.7726	1.7623
70	16.05	14.259	2.5724
80	18.05	16.036	2.8934
90	25.00	22.210	4.0098

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Temperatures were maintained using a thermostat bath with continuous stirring. Partial pressures of chlorobenzene were determined over 2 liter aqueous solutions in a flask. The equilibrium chlorobenzene content of the vapor was calculated from the gas laws. The amount of water vapor was obtained from the total weight increase of the absorber less the weight of the chlorobenzene absorbed. The chlorobenzene vapor pressure was directly proportional to its content in water. Duplicate measurements were made at each temperature.

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Source not specified, $n_D^{20} = 1.5248$, b.p. = 132°C

H_2O: Redistilled before use.

ESTIMATED ERROR:

Solubility: ±4%.

Temperature: ±0.1 K.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Högfeldt, E.; Bolander, B. *Ark. Kemi* 1963, *21(16)*, 161-86.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	5.40	3.0	3.06

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 15 ml chlorobenzene with 10 ml distilled water was shaken in a glass-stoppered bottle overnight at room temperature. After centrifugation, duplicate samples were taken for the determination of the water content in the organic phase. Titration of the samples was carried out by a modified Karl Fischer method (1). A small correction was made for water in the vapor phase and adsorbed on the pipet.

SOURCE AND PURITY OF MATERIALS:

H_2O: Distilled.

C_6H_5Cl: Source not specified, purity: 99.8%, impurity: 0.11% benzene.

ESTIMATED ERROR:

Solubility: ±10%.

Temperature: ±0.3 K.

REFERENCES:

1. Johansson, A. *Sven. Papperstidn.* 1947, *50(11B)*, 124-33.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Jones, J. R.; Monk, C. B. *J. Chem. Soc.* 1963, Part III, 2633-5.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10ml(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	3.4	1.88	1.92
30	3.95	2.182	2.239
35	4.6	2.54	2.62

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Tritiated water was shaken with chlorobenzene in 1:10 volume ratios for 4 hours in flasks placed in a water thermostat bath. The water content was determined by tritium assay of samples taken from the flasks. The count rates were determined using a typical liquid scintillator solution technique.

SOURCE AND PURITY OF MATERIALS:

H_2O: Tritiated.

C_6H_5Cl: 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) Chlorobenzene; C_6H_5Cl; [108-90-7]	Goldman, S., Ph.D. Dissertation, McGill University, Montreal, 1969, p. 84.
VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	5.225	2.90	2.959
35.1	7.405	4.11	4.234
45.06	9.639	5.35	5.567

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibration 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.

SOURCE AND PURITY OF MATERIALS:

H_2O: Distilled.

C_6H_5Cl: Reagent grade, washed with conc. H_2SO_4 and with 1 M $NaHCO_3$ and then fractionally distilled over silica gel.

ESTIMATED ERROR:

Solubility: ±2%.

Temperature: ±0.1 K.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Chey, W.; Calder, G. V. *J. Chem. Eng. Data* 1972, *17(2)*, 199-200.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10g(1)/kg(2) [a]	10^3mol(1)/kg [b]	$10^5 x(1)$ [c]
21	5.34	4.742	8.546

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 1 to 50 volume ratio solute/solvent mixture was stirred in a separatory funnel for 20 hr in a thermostat bath. Then, the solution was passed through a separation column of nonpolar resin. The solute was eluted with isopropyl ether. Traces of water were removed using molecular sieve pellets, and the sample was injected into a gas chromatograph fitted with a stainless steel column packed with Chromosorb having a liquid phase of Carbowax for analysis. The determination was done in duplicate.

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Source not specified, Analytical Reagent grade.

H_2O: Distilled.

ESTIMATED ERROR:
Solubility: ±2%.
Temperature: ±1 K.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg$ [a]	$10^3 mol(1)/kg(2)$ [b]	$10^5 x(1)$ [a]
25.0	4.622	4.108 ± 0.062	7.4004

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solute was equilibrated with water by stirring in a sealed flask (1) with a magnetic stirrer for 48 hours at constant temperature. A sample was withdrawn and filtered through a glass-wool plug and the solute was extracted with 2,2,4-trimethylpentene. The optical densities were determined spectrophotometrically (2). The mean and standard deviation were obtained from eight independent measurements.

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Merck AG., >99% GLC, used as received.

H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:

Solubility: ±1.51%.

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:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10g(1)/kg [a]	10^3mol(1)/kg(2) [b]	$10^5 x$(1) [a]
25.0	4.624	4.11	7.404

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium between the water and chlorobenzene was established by stirring the sample in a sealed flask (1) with a magnetic stirrer for 48 hours. The sample was filtered through a glass-wool plug and the chlorobenzene was extracted with 2,2,4-trimethylpentene. The optical density was determined spectrophotometrically (2). Five parallel determinations were made.

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

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: 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: ±1.7%.

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:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Prosyanov, N. N.; Shalygin, V. A; Zel'venskii, Ya. D. *Tr. Mosk. Khim. Tekhnol. Inst.* 1974, *81*, 55-6.
VARIABLES: Temperature: 298-361 K	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$$\log_{10}\alpha = \frac{1222.37}{T(K)} - 1.3225$$

where α = distribution coefficient.

At the normal boiling point of C_6H_5Cl: α = 49.0.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The water concentration in the saturated solutions was determined radiometrically using tritium labelled water.

The method of investigation has been described in greater detail in (1).

SOURCE AND PURITY OF MATERIALS:

H_2O: Not specified.

C_6H_5Cl: Not specified.

ESTIMATED ERROR:
Solubility: ±10% (compiler).

Temperature: ±0.5 K (compiler).

REFERENCES:

1. Prosyanov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D. *Tr. Mosk. Khim. Tekhnol. Inst.* 1973, *75*, 100-2.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* 1976, *54(24)*, 3909-16.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	5.225	2.90	2.959

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 50 ml chlorobenzene 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).

SOURCE AND PURITY OF MATERIALS:

H_2O: Distilled and deionized.

C_6H_5Cl: Fischer - B255, washed with cc. H_2SO_4 and K_2CO_3 solutions 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) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Nelson, H. D.; Smit, J. H. *S.-Afr. Tydskr. Chem.* 1978, *31(2)*, 76.
VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
5	0.400	0.355	0.64
25	1.068	0.9492	1.71
35	2.674	2.376	4.28
45	4.005	3.558	6.41

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated with chlorobenzene from the vapor phase in a special flask (1) placed in a thermostat bath using a shaker for a 24 hour equilibration period. A gas chromatographic analysis was done by sample injection into a 1.5 m stainless steel column having a 5% Apiezon M coating on Celite operated at 120°C. The chromatograph was fitted with a flame ionization detector. Three samples from each flask were analyzed.	C_6H_5Cl: Not specified. H_2O: Not specified.
	ESTIMATED ERROR: Solubility: ±2.9% (compiler). Temperature: ±0.1 K (compiler).
	REFERENCES: 1. Nelson, H. D.; de Ligny, C. L. *Rec. Trav. Chim.* 1968, *87*, 528-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Aquan-Yuen, M.; Mackay, D.; Shiu, W. Y. *J. Chem. Eng. Data* 1979, *24(1)*, 30-4.
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	4.717	4.1907	7.5753

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of solute was added to pure water in a flask which was then placed in a constant temperature bath for equilibration for at least 48 hours before analysis. The concentration of the chlorobenzene was determined by solvent extraction, followed by gas chromatographic analysis. The chromatograph was equipped with a flame ionization detector as described in (1).

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: Fisher Scientific Inc., certified grade, used as received.

H_2O: Specified as "pure".

ESTIMATED ERROR:

Solubility: ±3.8%.

Temperature: ±0.5 K (evaluator).

REFERENCES:

1. Mackay, D.; Shiu, W. Y. *Bull. Environ. Contam. Toxicol.* 1976, *15*, 101-12.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Schwarz, F. P.; Miller, J. *Anal. Chem.* 1980, *52(13)*, 2162-4.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

Experimentally determined values:

t/°C	10g(1)/kg Elution Chromatography	UV Absorption
10.0	4.4 ± 0.2	4.9 ± 0.3
20.0	4.2 ± 0.2	4.8 ± 0.4
30.0	4.9 ± 0.1	5.0 ± 0.2

Values derived from average measured solubilities:

t/°C	10g(1)/kg [a]	10^3mol(1)/kg [b]	$10^5 x(1)$ [c]
10.0	4.6 ± 0.2	4.09 ± 0.18	7.37 ± 0.32
20.0	4.5 ± 0.4	4.00 ± 0.36	7.21 ± 0.64
30.0	5.0 ± 0.1	4.44 ± 0.09	8.01 ± 0.16

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 upon liquid phase elution chromatography has been described in (1).

SOURCE AND PURITY OF MATERIALS:

C_6H_5Cl: 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:	ORIGINAL MEASUREMENTS:
(1) Water-d_2; D_2O; [7729-20-0] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Hutchison, C. A.; Lyon, A. M. Columbia University Report A-745, July 1, 1943.
VARIABLES:	PREPARED BY:
One temperature	G. Jancso

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^3 x(1)$ [a]
25.0	4.386	2.19	2.460

a. Calculated by F. W. Getzen.
b. Reported (average of two experimental measurements).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Between 25 and 100 ml of chlorobenzene and 1 to 2 ml of D_2O were introduced into a flask and shaken for about 90 min. The water bath temperature was maintained within ±0.05°C. Then, a sample was taken and the dissolved D_2O content was determined by a modified Karl Fischer titration as described in (1).

The original report was unavailable, but the method and results have been described in sufficient detail in (1). The solubility of H_2O in chlorobenzene was also determined and found to be 0.00250 ± 0.00003 mol H_2O/100 g solution from three separate experiments.

SOURCE AND PURITY OF MATERIALS:

Chlorobenzene was carefully purified and dried before use. Source and method not given.

100% D_2O: Source not specified.

ESTIMATED ERROR:

Solubility: av. dev. ±1 x 10^{-5} mol D_2O/100 g solution.

Temperature: ±0.05 K.

REFERENCES:

1. Eidinoff, M. L. In "Production of Heavy Water", National Nuclear Energy Series Division III-Vol. 4F, Murphy, G. M.; Urey, H. C.; Kirshenbaum, I.; Eds.; McGraw-Hill: New York, 1955; Part II, Chapter 7, pp 129-44.