COMPONENTS:	EVALUATOR:
(1) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION:

The solubility of 1,2,4-trichlorobenzene in water has been measured by Meleshchenko (1), Yalkowsky et al. (2), and Chiou et al. (3). However, there appears to be a serious discrepancy between the three reported solubility values. According to the authors, the error estimates in their measurements were ± 8 percent for Meleshchenko, ± 10 percent for Yalkowsky et al., and ± 5 percent for Chiou et al. Consequently, in view of these uncertainties, the recommended solubility value must be taken as the arithmetical mean for the three reported measured values.

With reference to Figures 3 and 4 in the Introduction, the recommended solubility of 1,2,4-trichlorobenzene in water given below for 298.15 K is within an acceptable margin of expectation.

The single data point available for the solubility of water in 1,2,4-trichlorobenzene at 298.15 K by Eidinoff (4) is accepted as a tentative value.

T/K	10^3mol(1)/dm^3	10^2g(1)/kg	10^4x(1)
298.15	3.05	3.79	3.82

T/K	10^2mol(2)/dm^3	10g(2)/kg	10^3x(2)
298.15	1.63	2.02	2.03

REFERENCES

1. Maleshchenko, K. F. *Gigiena i Sanit.* 1960, *25(5)*, 54-57.

2. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

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

4. 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) Water; H_2O; [7732-18-5] (2) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]	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.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10g(1)/kg [a]	10^2mol(1)/kg [b]	10^3x(1) [a]
25	2.0232	1.123	2.0340

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Addition of 2 ml H_2O to 100 ml $C_6H_3Cl_3$ in an equilibration flask was performed in a dry box. The closed flask was then placed in a water thermostat bath and the assembly was shaken for 90 min. The samples for analysis were taken with a sampling pipet while the equilibrium temperature was maintained. The water content in the sample was determined by a modified Karl Fischer titration.

SOURCE AND PURITY OF MATERIALS:

$C_6H_3Cl_3$: Purified and dried before use.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: Average dev. ±0.00006 mol(1)/kg.

Temperature: ±0.05 K.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1] (2) Water; H_2O; [7732-18-5]	Maleshchenko, K. F. *Gigiena i Sanit.* 1960, *25(5)*, 54-57.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10^2g(1)/dm^3 [a]	10^4mol(1)/dm^3 [b]	$10^6 x$(1) [c]
19	3.0	1.65	2.98

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A 100 mg trichlorobenzene in 1 liter water mixture was shaken periodically for 5 days at 18-20°C. After filtration, a determined quantity of ether was added and extracted three times. The ether was evaporated and oxidation of the residue was accomplished with chlorosulphonic acid. The chlorine content was determined by iodometric titration.	$C_6H_3Cl_3$: Not specified. H_2O: Twice distilled before use.
	ESTIMATED ERROR: Solubility: ±8%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10^2g(1)/dm^3 [a]	10^4mol(1)/dm^3 [b]	$10^6 x$(1) [a]
25	3.466	1.91	3.451

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A small excess of 1,2,4-trichlorobenzene in water was agitated at room temperature for about 24 hours and then filtered. The filtrate was diluted and assayed spectrophotometrically. The determination was carried out in duplicate.

SOURCE AND PURITY OF MATERIALS:

$C_6H_3Cl_3$: Aldrich commercial grade, used as received.

H_2O: Deionized.

ESTIMATED ERROR:
Solubility: ±10%.

Temperature: ±1 K.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1] (2) Water; H_2O; [7732-18-5]	Chiou, C. T.; Schmedding, D. V.; Manes, M. *Environ. Sci. Technol.* 1982, *16(1)*, 4-10.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10^2g(1)/dm^3 a	10^4mol(1)/dm^3 b	10^6x(1) a
25	4.881	2.69	4.861

Note: The solubility was also reported in (1), as "unpublished results".

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of 1,2,4-trichlorobenzene 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:

$C_6H_3Cl_3$: Not specified.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±5% (compiler).

Temperature: ±0.5 K.

REFERENCES:

1. Chiou, C. T. *Hazard Assess. Chem. Current Dev.* 1981, *1*, 117-53.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water-d_2; D_2O; [7789-20-0] (2) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]	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]	10^3mol(1)/kg [b]	10^3x(1) [a]
25.0	1.999	9.98	1.808

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Between 25 and 100 ml 1,2,4-trichlorobenzene and 1 to 2 ml D_2O were placed in a flask and shaken for about 90 min. The thermostat water bath temperature was maintained within ±0.05°C. Then, a sample was removed and the amount of D_2O dissolved was determined by a modified Karl Fischer titration (1).

The original report was unavailable; however, the method and the results were described in sufficient detail in (1). The solubility of H_2O in 1,2,4-trichlorobenzene was also determined and found to be 0.01123 mol(1)/kg. The average deviation for two experiments was ±0.00006 mol(1)/kg.

SOURCE AND PURITY OF MATERIALS:

$C_6H_3Cl_3$: Carefully purified and dried before use. Source and method not given.

D_2O: Source not specified.

ESTIMATED ERROR:

Solubility: av. dev. ±2.1 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.