COMPONENTS:	EVALUATOR:
(1) Iodobenzene; C_6H_5I; [591-50-4]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION:

Five experimental determinations have been published on the solubility of iodobenzene in water in the temperature interval between 278 and 318 K (1-4,8), see Figure 1. The serious discrepancies between the various solubility measurements for iodobenzene in water are evident in Figure 1. The solubility of water in iodobenzene between 298 and 308 K has been reported in two publications (5,6), see Figure 2.

Some of the more recent data for the solubility of iodobenzene in water is that of Nelson and Smit (3) 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 (7). Consequently, for the present evaluation, their results have not been considered for inclusion in the selected solubility values.

The solubility value for iodobenzene in water reported by Gross et al. (2) is too high in relation to other reported values (1,4). While the equilibration time was 20 hours for measurements made by Andrews and Keefer (1), the time was 48 hours for those of Vesala (4). This equilibration time difference may have affected the reported results. For this reason, the higher solubility value given by Vesala is recommended, see Table 1. The remaining available data have been correlated relative to Absolute temperature using a normal polynomial equation:

$$S_1(g)1)/kg) = 0.59293 - 4.8616 \times 10^{-3}T + 1.21754 \times 10^{-5}T^2 \quad [1]$$

The values calculated from equation [1] for the saturation of iodobenzene in water in the range of temperatures between 283 and 318 K together with corresponding molarities and mole fractions are given 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.

For the solubility of water in iodobenzene, the agreement between the two solubilities reported by Jones and Monk (5) and by Wing and Johnston (6) at 298.15 K is quite good. At higher temperatures, measurements were made only by Jones and Monk (5); therefore, there are no other data for comparison. The data from both investigations (5,6) were correlated using the following equation:

$$\log_{10} x(2) = 0.792324 - 985.707/T \quad [2]$$

In this equation, $x(2)$ is the mole fraction solubility of water in the water-iodobenzene system and T is the Absolute temperature. The calculated solubility values in the 283 to 308 K range are shown in Figure 2 along with the reported values.

The calculated mole fraction values for the solubility of water in iodobenzene from equation [2] are included in Table 2 together with the corresponding molarities and g(2)/kg values in the temperature range between 293 and 313 K.

COMPONENTS:	EVALUATOR:
(1) Iodobenzene; C_6H_5I; [591-50-4]	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 Iodobenzene in Water.

T/K	10^4mol(1)/dm^3	10g(1)/kg	10^5x(1)
283.15	9.43	1.93	1.70
288.15	9.94	2.03	1.79
293.15	10.5	2.14	1.89
298.15	11.0	2.26	1.99
303.15	11.6	2.38	2.10
308.15	12.2	2.51	2.22
313.15	12.9	2.64	2.34
318.15	13.5	2.79	2.46

Table 2. Solubility of Water in Iodobenzene.

T/K	10^2mol(2)/dm^3	10g(2)/kg	10^3x(2)
293.15	2.42	2.38	2.69
298.15	2.74	2.71	3.06
303.15	3.10	3.08	3.47
308.15	3.49	3.48	3.92
313.15	3.90	3.91	4.41

REFERENCES

1. Andrews, L. J.; Keefer, R. J. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.
2. Gross, P. M.; Saylor, J. H.; Gorman, M. A. *J. Am. Chem. Soc.* 1933, *55(2)*, 650-2.
3. Nelson, H. D.; Smit, J. H. *S.-Afr. Tydskr. Chem.* 1978, *31(2)*, 76.
4. Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.
5. Jones, J. R.; Monk, C. B. *J. Chem. Soc.* 1963, *Part III*, 2633-5.
6. Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.
7. Nelson, H. D., Personal Communication, 1979.
8. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.

COMPONENTS:	EVALUATOR:
(1) Iodobenzene; C_6H_5I; [591-50-4]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979.

CRITICAL EVALUATION: (Continued)

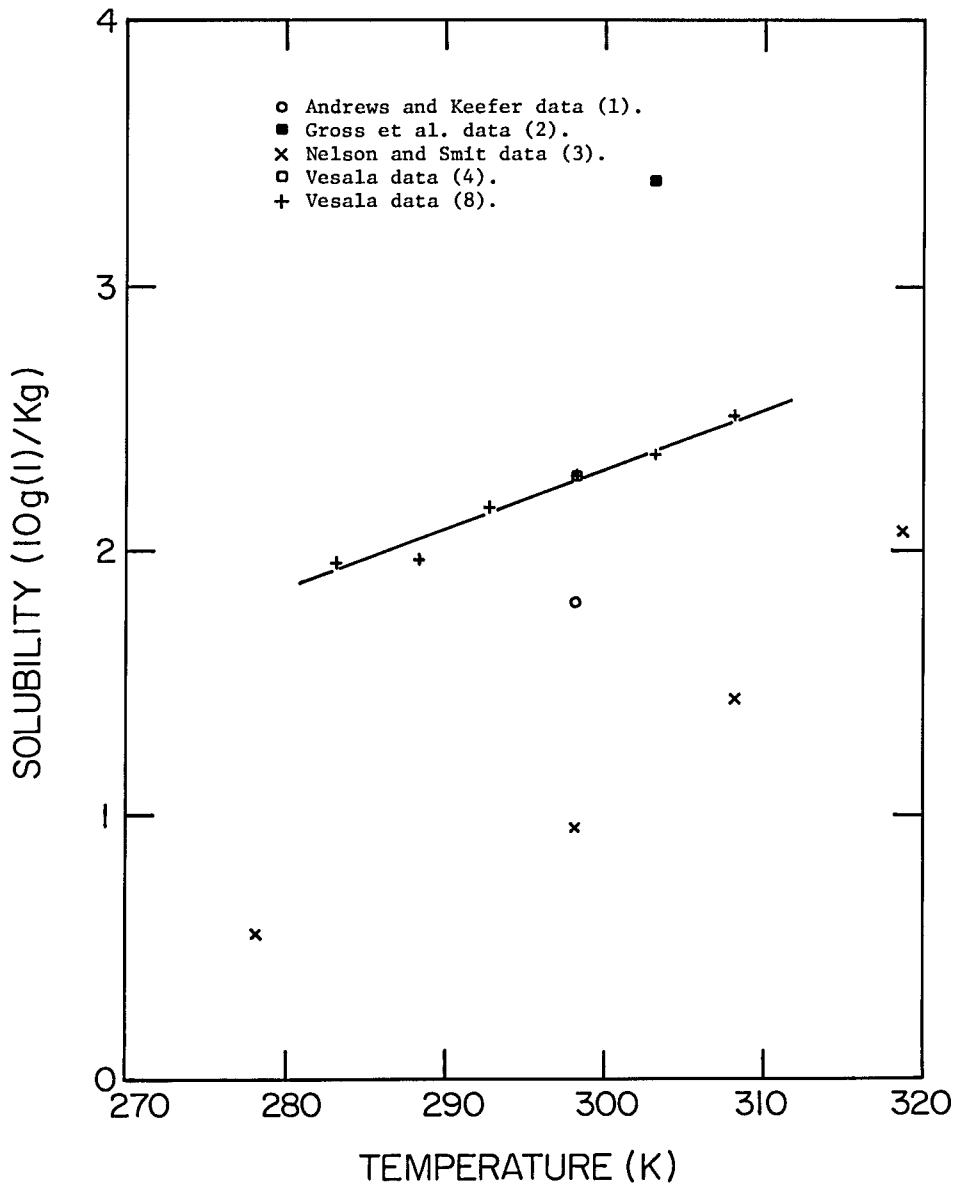

Figure 1. Solubility of iodobenzene in water versus Absolute temperature, reported and calculated values.

COMPONENTS:	EVALUATOR:
(1) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Iodobenzene; C_6H_5I; [591-50-4]	May 1979.

CRITICAL EVALUATION: (Continued)

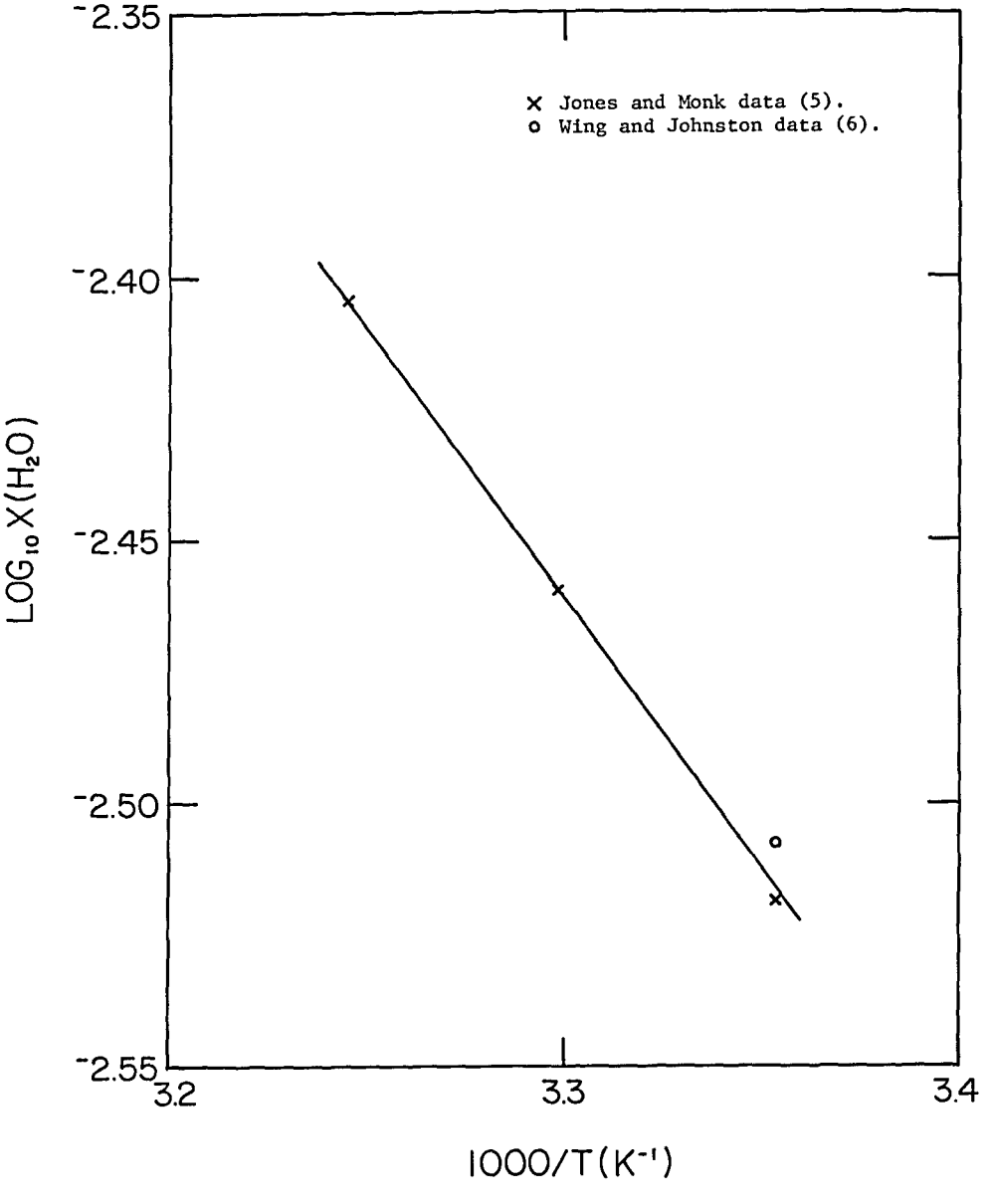

Figure 2. Logarithm of mole fraction solubility of water in iodobenzene versus reciprocal of Absolute temperature, reported and calculated values.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	Gross, P. M.; Saylor, J. H.; Gorman, M. J. *J. Am. Chem. Soc.* 1933, *55(2)*, 650-2.
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]
30	3.4	1.67	3.00

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solution was prepared in a thermostat water bath. The samples were analyzed by means of a Zeiss combination liquid and gas interferometer described in (1). A detailed description of the complete procedure has been included in a M.A. thesis (2).

SOURCE AND PURITY OF MATERIALS:

C_6H_5I: Eastman Kodak Co., distilled fractionally before use, b.p. range 84.55° - 84.63°C.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±4%.

Temperature: ±0.02 K.

REFERENCES:

1. Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* 1931, *53(5)*, 1744-51.
2. Gorman, M. A., M. A. thesis, Duke University, Durham, 1932.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.
VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25.0	1.8	8.82	1.59

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water was saturated with iodobenzene 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_5I: Eastman Kodak Co., commercial reagent, b.p. 188.3°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) Iodobenzene; C_6H_5I; [591-50-4]	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	$10ml(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	5.03	2.784	3.107

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Tritiated water was equilibrated with 20 ml iodobenzene 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_5I: Source not specified, chemical grade, redistilled before use.

ESTIMATED ERROR:
Solubility: ±1.6%.

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) Iodobenzene; C_6H_5I; [591-50-4]	Jones, J. R.; Monk, G. B. *J. Chem. Soc.* 1963, *Part III*, 2633-5.
VARIABLES:	PREPARED BY:
Temperature	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	4.9	2.71	3.03
30	5.6	3.09	3.47
35	6.35	3.502	3.940

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 iodobenzene 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 scintillatior solution technique.	H_2O: Tritiated. C_6H_5I: 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) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	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]	10^3mol(1)/kg(2) [b]	$10^5 x(1)$ [a]
10.0	1.9529	0.9574 ± 0.0093	1.7248
15.2	1.9656	0.9636 ± 0.0084	1.7360
19.6	2.1642	1.061 ± 0.033	1.9115
25.1	2.2845	1.120 ± 0.032	2.0177
30.0	2.3620	1.158 ± 0.026	2.0862
35.0	2.5109	1.231 ± 0.007	2.2177

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The iodobenzene 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_5I: Flika AG, puriss, >99% GLC, used as received.

H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:
Solubility: ±3.11%.

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) Iodobenzene; C_6H_5I; [591-50-4] (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]	10^5x(1) [a]
25.0	2.2845	1.120	2.0177

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The iodobenzene 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 established from five parallel determinations.

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

SOURCE AND PURITY OF MATERIALS:

C_6H_5I: 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: ±2.7%.

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) Iodobenzene; C_6H_5I; [591-50-4] (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]	10^4mol(1)/kg [b]	$10^6x(1)$ [c]
5	0.5492	2.692	4.85
25	0.9500	4.657	8.39
35	1.438	7.048	12.7
45.5	2.072	10.16	18.3

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water was saturated through the vapor phase with iodobenzene in a special flask (1) using a shaker in a thermostat bath for 24 hours. A gas chromatographic analysis of the samples was done by injection into a 5% Apiezon M stainless steel column with Celite as the supporter. The column length was 1.5 m and the temp. was 120°C. The chromatograph was equipped with a flame ionization detector. Three samples were analyzed from each flask.

SOURCE AND PURITY OF MATERIALS:

C_6H_5I: Not specified.

H_2O: Not specified.

ESTIMATED ERROR:

Solubility: ±2% (compiler).

Temperature: ±0.1 K (compiler).

REFERENCES:

1. Nelson, H. D.; de Ligny, C. L. *Rec. Trav. Chim.* 1968, *87*, 528-44.