COMPONENTS:	EVALUATOR:
(1) 1,4-Diiodobenzene; $C_6H_4I_2$; [624-38-4] (2) Water; H_2O; [7732-18-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku. September 1979.

CRITICAL EVALUATION:

Two experimental values have been reported for the solubility of 1,4-diiodobenzene in water, that determined by Andrews and Keefer (1) and a recent one measured by Yalkowsky, Orr, and Valvani (2). The former study deals with the argentation of substituted benzenes and the latter work presents some useful correlations for the solubilities of halogenated benzenes in water.

The analytical procedure used by Andrews and Keefer is, in principle, quite adequate for the purpose; however, the time for saturation equilibration seems to have been too short and no tests for reaching saturation equilibria were presented (3). Furthermore, the melting point of 360-361 K reported for 1,4-diiodobenzene deviates considerably from reported literature values of 402-403 K (4a,4b). Whether this difference resulted from impurities or from some other cause is difficult to establish.

The saturation equilibrium periods for the measurements of Yalkowsky et al. also seem rather short. The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. A conventional experimental procedure was employed in their measurements. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (5), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The value reported by Yalkowsky et al. appears to be more reliable than that of Andrews and Keefer. Therefore, the value of Yalkowsky et al. is reported here as a tentative solubility of 1,4-diiodobenzene in water:

T/K	10^6mol(1)/dm^3	10^3g(1)/kg	$10^7x(1)$
298.15	5.6	1.85	1.01

REFERENCES

1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.
2. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
3. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1949, *71(11)*, 3644-7.
4. a. Paulsen, O. *Monatsh. Chem.* 1939, *72*, 254.
   b. "Handbook of Tables for Organic Compound Identification", 3rd ed.; Rappoport, Z., Compiler; CRC Press: Cleveland, Ohio, 1967; p. 76.
5. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:

(1) 1,4-Diiodobenzene; $C_6H_4I_2$; [624-38-4]

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

ORIGINAL MEASUREMENTS:

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

VARIABLES:

One temperature

PREPARED BY:

A. Vesala

EXPERIMENTAL VALUES:

t/°C	$10^3 g(1)/dm^3$ [a]	$10^6 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	1.85	5.6	1.01

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A small excess of solute in water was agitated for a period of 4 - 48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was diluted and assayed spectrophotometrically. At least two independent determinations were carried out.

SOURCE AND PURITY OF MATERIALS:

$C_6H_4I_2$:	Commerical reagent (Aldrich or Eastman), used as received.
H_2O:	Source and purity not reported.

ESTIMATED ERROR:

Solubility: ±10% (authors).

Temperature: ±1 K (authors).

REFERENCES:

COMPONENTS:

(1) 1,4-Diiodobenzene; $C_6H_4I_2$; [624-38-4]

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

ORIGINAL MEASUREMENTS:

Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.

VARIABLES:

One temperature

PREPARED BY:

A. Vesala

EXPERIMENTAL VALUES:

t/°C	$10^3 g(1)/dm^3$ a	$10^6 mol(1)/dm^3$ b	$10^8 x(1)$ b
25.0	1.4	4.24	7.67

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturation process was done in sealed Erlenmeyer flasks. The time used for the equilibration was 20 hours. Measured volumes of the saturated solution were then extracted using measured volumes of hexane to remove the aromatic compound from the aqueous layer. The solute concentration was measured spectrophotometrically (1).

SOURCE AND PURITY OF MATERIALS:

$C_6H_4I_2$:	Commercial product (Eastman Kodak Co.), recrystallized twice from ethanol, reporting melting point 360-361 K.
H_2O:	Source and purity not specified.

ESTIMATED ERROR:

Solubility: >10% (compiler).

Temperature: ± 0.2 K.

REFERENCES:

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