COMPONENTS:	EVALUATOR:
(1) 1,4-Dibromobenzene; $C_6H_4Br_2$; [106-37-6] (2) Water; H_2O; [7732-18-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku. January 1979

CRITICAL EVALUATION:

There are only a few reported measurements dealing with the solubility of 1,4-dibromobenzene in water. In the published papers on the subject, the determination of solubility is not the primary purpose of the work, a fact that may affect the precision of the reported results. Of the values reported, only that of Andrews and Keefer (1) refers to 298.2 K. The measured data reported by Hine, Haworth, and Ramsay (2) at 308.2 K lend some support to the value assigned at 298.2 K.

The experimental procedure employed by Andrews and Keefer is adequate for the determination in question. However, the time of equilibrium (about 20 hours as given in (3)) seems quite short in the absence of tests for solution equilibrium. It is reasonable to attribute most of the uncertainty in the reported solubility of 8.5 x 10^{-5} mol(1)/dm^3 (7.0 x 10^{-5} molar at an ionic strength of 1.0 molar, a figure incorrectly cited for solubility in pure water in some papers). Support for the reliability of the value at 298.2 K is provided by the value of 1.12 x 10^{-4} mol(1)/kg(2) given by Hine et al. for 308.2 K. This value was obtained by employing a long equilibration (at least a week) and a direct spectrophotometric measurement. In fact, it seems reasonable that the latter measurements should be more reliable than those of Andrews and Keefer although the agreement between the two measurements is quite satisfactory. The increase in the solubility is about 30% for a temperature rise of 10 degrees from 298.2 K. This increase is about the same magnitude as that for 1,4-dichlorobenzene in water in the same range of temperature as measured by Wauchope and Getzen (4).

The following is the tentative solubility of 1,4-dibromobenzene in water at 298.15 K:

T/K	10^5mol(1)/dm^3	10^2g(1)/kg	$10^6x(1)$
298.15	8.5	2.0	1.5

REFERENCES

1. Andrews, L. M.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.
2. Hine, J.; Haworth, H. W.; Ramsay, O. B. *J. Am. Chem. Soc.* 1963, *85(10)*, 1473-6.
3. Andrews, L. M.; Keefer, R. M. *J. Am. Chem. Soc.* 1949, *71(11)*, 3644-7.
4. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dibromobenzene; $C_6H_4Br_2$; [106-37-6] (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. Vesala

EXPERIMENTAL VALUES:

t/°C	$10^2 g(1)/dm^3$ a	$10^5 mol(1)/dm^3$ b	$10^6 x(1)$ b
25.0	2.0	8.48	1.53

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 solutions were then extracted using measured volumes of hexane to remove the aromatic matter from the aqueous layer. The solute concentration was measured spectrophotometrically using a Beckman DU spectrophotometer (1).

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Br_2$:	Commercial product (Eastman Kodak Co.), used as received.
H_2O:	Source and purity not specified.

ESTIMATED ERROR:

Solubility: >10% (evaluator).

Temperature: ±0.2 K (evaluator).

REFERENCES:

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

COMPONENTS:

(1) 1,4-Dibromobenzene; $C_6H_4Br_2$; [106-37-6]

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

ORIGINAL MEASUREMENTS:

Hine, J.; Haworth, H. W.; Ramsay, O. B. *J. Am. Chem. Soc.* 1963, *85(10)*, 1473-6.

VARIABLES:

One temperature

PREPARED BY:

A. Vesala

EXPERIMENTAL VALUES:

t/°C	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
35.0	2.642	1.12	2.030

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of the aromatic compound was combined with 4.0 ml of water in a 5.0 ml ampoule which was then sealed. The sealed ampoule was rotated in a constant temperature water bath for at least a week to establish saturation. The undissolved solid was removed by filtration and the concentration of the solute in the saturated filtrate solution was determined by ultraviolet spectrophotometric measurements using a Beckman DU spectrophotometer. Several measurements were taken at intervals of at least a day in order to be sure that an equilibrium had been established.

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Br_2$:	Source not specified; presumably commercial material, recrystallized to constant melting point in agreement with literature values.
H_2O:	Source and purity not specified.

ESTIMATED ERROR:

Solubility: ±7% (standard deviation reported by authors).

Temperature: ±0.1 K (authors).

REFERENCES: