COMPONENTS:	EVALUATOR:
(1) Pentachlorobenzene; C_6HCl_5; [608-93-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	September 1982.

CRITICAL EVALUATION:

The solubility of pentachlorobenzene in water has been measured by Yalkowsky, Orr, and Valvani (1) and by Banerjee, Yalkowsky, and Valvani (2). The measurements differ primarily in the analytical procedures involved. The principal motivation for the studies was to obtain certain correlations for solubilities of halogenated benzenes in water.

In the former measurements (1), a conventional experimental procedure was employed. Commercial reagents without further purification were used for the measurements which were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. 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 (3), 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 latter investigation (2) was based upon a radiochemical analysis. Although temperature regulation and time for equilibration seemed to have received sufficient attention, the result deviates far more than 10 percent from the value reported in (1). The accuracy of the latter measurements also depends upon the radiochemical purity of the substrate, a property which was not tested. The uncertainty of radiochemical purity may account in part for the deviation from the spectrophotometrically determined value.

The solubility of pentachlorobenzene in water is reported here as a tentative value based upon the spectrophotometric determinations (1):

T/K	10^6mol(1)/dm^3	10^4g(1)/kg	$10^8 x$(1)
298.15	2.2	5.52	3.95

REFERENCES

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

2. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* 1980, *14(10)*, 1227-9.

3. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorobenzene; C_6HCl_5; [608-93-5] (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: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

t/°C	10^4 g(1)/dm^3 [a]	10^6 mol(1)/dm^3 [b]	$10^8 x$(1) [a]
25	5.51	2.2	3.95

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 extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.

SOURCE AND PURITY OF MATERIALS:

C_6HCl_5: Commercial reagent (Aldrich or Eastman), used as received.

H_2O: Source and purity not specified.

ESTIMATED ERROR:

Solubility: ±10% (authors).

Temperature: ±1 K (authors).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorobenzene; C_6HCl_5; [608-93-5] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Techn.* 1980, *14(10)*, 1227-9.
VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

t/°C	10^3g(1)/dm^3 [a]	10^6mol(1)/dm^3 [b]	$10^8 x$(1) [a]
25	1.332	5.32	9.613

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equilibrium was performed in sealed stainless steel centrifuge tubes with constant or intermittent shaking. The equilibrium was generally complete within 1 week. The mixture was then centrifuged for 60 minutes after which aliquots of the solution were removed for analysis either by a pipet or syringe. Liquid scintillation counting with ^{14}C-labelled solute was employed in the solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

C_6HCl_5: Commercial reagent, the ^{14}C-labeled compound was purchased by NEN, the nonlabeled one by Aldrich.

H_2O: Distilled water.

ESTIMATED ERROR:

Solubility: ±4.9% (std. deviation estimated by authors).

Temperature: ±0.2 K (equilibration)
±0.3 K (centrifugation).

REFERENCES: