

<p>COMPONENTS:</p> <p>(1) Hexachlorobenzene; C_6Cl_6; [118-74-1]</p> <p>(2) Water; H_2O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>A. Vesala, Department of Chemistry and Biochemistry, University of Turku</p> <p>September 1982</p>
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CRITICAL EVALUATION:

Little is known about the solubility of hexachlorobenzene in water at normal temperatures despite the fact that large quantities of this compound are used commercially. In recent times, however, toxicologists and environmental chemists have begun to study the aqueous solubilities of chlorinated aromatic hydrocarbons in connection with pollution analyses. Currently, solubility data for this compound at ordinary temperatures exist in two published papers. A third work reports the solubility of hexachlorobenzene at higher temperatures.

The work of Weil, Dure, and Quentin (1) discusses the determination of extremely small solubilities. Their saturation process was carried out by a chromatographic technique to avoid contamination on glass surfaces and formation of possible colloidal aggregates of the solute. In their procedure, Mg silica gel, overcoated with the solute, was eluted with water. However, the analytical procedure was not reported, a factor which makes it difficult to estimate the precision of the measured values. It is known that certain problems and complications arise in the course of the determination of solubilities of this magnitude. First of all, the effects of a third component (glass or silica gel) may be significant. Also, the purity of the solvent (water) can exert a dominant influence on results in cases of highly diluted, saturated systems. In addition to distillation and deionization, the solvent should also be degassed, a procedure not done for the reported measurements. For such reasons, the values of Weil et al. may involve large absolute errors.

Hollifield (2) applied a nephelometric procedure for the estimation of the solubility of hexachlorobenzene in water. His analytical method involved the preparation of a standard curve by successive dilution of an acetone solution of the test substance with water. The turbidities of the solutions were measured nephelometrically. Extrapolation of this curve to an intensity of the reagent blank gave an estimate of the solubility in water. The solubility value reported for 297 ± 2 K was $110 \mu\text{g}(1)/\text{kg}$. The method evidently gives rough estimates of the solubilities and it has the advantage of being rapid. The lack of precision in the procedure can be appreciated from a review of the reported solubility data which show deviations of several orders of magnitude from reported literature values. Consequently, these solubility values are not considered further in this evaluation.

Sharov (3) has reported the solubility of hexachlorobenzene in water at higher temperatures. Two variables (temperature and pressure) make a comparison with other solubility data difficult. Only the value referred to 353 K was probably measured at normal pressure. Even so, its value of $10 \text{ mg}(1)/\text{kg}(2)$ cannot be used to support the solubility value of Weil et al.

The following solubility value for hexachlorobenzene in water is based upon the value reported by Weil et al. However, for the reasons stated, the value should be considered doubtful.

T/K	$10^8 \text{ mol}(1)/\text{dm}^3$	$10^6 \text{ g}(1)/\text{kg}$	$10^{10} x(1)$
298.15	1.8	5.0	3.2

REFERENCES

1. Weil, L.; Dure, G.; Quentin, K-E. *Wasser Abwasser Forsch.* 1974, *7*, 169-75.
2. Hollifield, H.C. *Bull. Environ. Contam. Toxicol.* 1979, *23(4/5)*, 579-86.
3. Sharov, V. G. *V. Sb. Dostizheniya Nauk-Neftekhim-Vam.* 1975, 138-41.

COMPONENTS: (1) Hexachlorobenzene; C_6Cl_6 ; [118-74-1] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Weil, L.; Dure, G.; Quentin, K-E. <i>Wasser Abwasser Forsch.</i> <u>1974</u> , 7, 169-75.								
VARIABLES: One temperature	PREPARED BY: A. Vesala								
EXPERIMENTAL VALUES: <table border="1" data-bbox="225 454 960 540"> <thead> <tr> <th>t/°C</th> <th>10^6 g(1)/dm^3 ^a</th> <th>10^8 mol(1)/dm^3 ^b</th> <th>$10^{10} x(1)$ ^b</th> </tr> </thead> <tbody> <tr> <td>25</td> <td>5.0</td> <td>1.76</td> <td>3.17</td> </tr> </tbody> </table> <p>a. Reported. b. Calculated by F. W. Getzen.</p>		t/°C	10^6 g(1)/dm^3 ^a	10^8 mol(1)/dm^3 ^b	$10^{10} x(1)$ ^b	25	5.0	1.76	3.17
t/°C	10^6 g(1)/dm^3 ^a	10^8 mol(1)/dm^3 ^b	$10^{10} x(1)$ ^b						
25	5.0	1.76	3.17						
AUXILIARY INFORMATION									
METHOD/APPARATUS/PROCEDURE: <p>The saturation process involved a chromatographic technique. A 600 mg Florisil powder sample (15.5% MgO, 84.0% SiO₂, 0.5% Na₂SO₄), 60/100 mesh, was overcoated with 10 mg solute in 10 ml acetone solution. After the acetone was removed by evaporation, the solid mixture was transferred to a column (5 mm diameter, 7 cm length) and the solute was eluted from the Mg silica gel coating with water. The organic solute was then extracted from the water solution. The procedure for determining the composition of the extracted sample was not specified.</p>	SOURCE AND PURITY OF MATERIALS: C_6Cl_6 : Source and purity not specified. H_2O : Twice distilled. ESTIMATED ERROR: Solubility: >20% (This evaluation is based on the table I in the original paper. In the table the effect of the ratio of the organic compound and Florisil was tested with five determinations in each case.) Temperature: ± 0.2 K (evaluator). REFERENCES:								