

<p>COMPONENTS:</p> <p>(1) 1,2,4,5-Tetrabromobenzene; C₆H₂Br₄; [636-28-2]</p> <p>(2) Water; H₂O; [7732-18-5]</p>	<p>EVALUATOR:</p> <p>A. Vesala, Department of Chemistry and Biochemistry, University of Turku.</p> <p>November 1979.</p>
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CRITICAL EVALUATION:

A single solubility measurement of 1,2,4,5-tetrabromobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature ($25 \pm 1^\circ\text{C}$). 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 (2), 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 solubility of 1,2,4,5-tetrabromobenzene in water is reported here as a tentative value:

T/K	$10^7 \text{ mol}(1)/\text{dm}^3$	$10^5 \text{ g}(1)/\text{kg}$	$10^9 x(1)$
298.15	1.1	4.34	1.99

REFERENCES

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

COMPONENTS: (1) 1,2,4,5-Tetrabromobenzene; $C_6H_2Br_4$; [636-28-2] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. <i>Ind. Eng. Chem. Fundam.</i> <u>1979</u> , <i>18(4)</i> , 351-3.								
VARIABLES: One temperature	PREPARED BY: A. Vesala								
EXPERIMENTAL VALUES: <table border="0" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left; padding-right: 20px;">$t/^\circ C$</th> <th style="text-align: left; padding-right: 20px;">$10^5 g(1)/dm^3$ ^a</th> <th style="text-align: left; padding-right: 20px;">$10^7 mol(1)/dm^3$ ^b</th> <th style="text-align: left;">$10^9 x(1)$ ^a</th> </tr> </thead> <tbody> <tr> <td style="text-align: left; padding-right: 20px;">25</td> <td style="text-align: left; padding-right: 20px;">4.33</td> <td style="text-align: left; padding-right: 20px;">1.1</td> <td style="text-align: left;">1.99</td> </tr> </tbody> </table> <p style="margin-left: 20px;">a. Calculated by F. W. Getzen. b. Reported.</p>		$t/^\circ C$	$10^5 g(1)/dm^3$ ^a	$10^7 mol(1)/dm^3$ ^b	$10^9 x(1)$ ^a	25	4.33	1.1	1.99
$t/^\circ C$	$10^5 g(1)/dm^3$ ^a	$10^7 mol(1)/dm^3$ ^b	$10^9 x(1)$ ^a						
25	4.33	1.1	1.99						
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: $C_6H_2Br_4$: Commercial product (Aldrich or Eastman), used as received. H_2O : Source and purity not specified. ESTIMATED ERROR: Solubility: $\pm 10\%$ (authors). Temperature: ± 1 K (authors). REFERENCES:								