

<p>COMPONENTS:</p> <p>(1) 2,3,4,6-Tetrachlorophenol; $C_6H_2Cl_4O$; [58-90-2]</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>November 1979.</p>
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CRITICAL EVALUATION:

One study has been reported in the literature concerning the solubility of 2,3,4,6-tetrachlorophenol in water by Blackman, Parke, and Garton (1). Their concern was the relation of physical properties of certain substituted phenols to their physiological activities. In order to standardize the measuring conditions, they regulated the pH of all their saturated solutions to a value of 5.1 by the slight addition of a phosphate buffer. The electrolytic effects of this buffer addition on the equilibrium solubility can be neglected. However, the effects of pH changes upon the solubility are more complicated and should not be overlooked. In order to establish the solubility behavior generally, one must measure solubilities with pH as one of the variables. Such data, however, do not exist for 2,3,4,6-tetrachlorophenol. The only alternative here is to consider the total solubility of the compound in water, considering total solubility as the sum of the concentrations of the phenol and the phenolate ion. In the final analysis, the overall influence of pH upon the solubility is controlled by the acidity constant of the 2,3,4,6-tetrachlorophenol which was reported to be 5.3 by Blackman et al. Evidently the regulation of pH to a value of 5.1 in this case provides a higher concentration of the phenolate ion relative to the undissociated phenol as compared to that in a solution simply saturated with the pure phenol. Thus, the solubility value at the pH of 5.1 should have a somewhat higher value than that for the saturated solution of the pure phenol.

The information concerning the purity and further treatment of the reagents was also incomplete. The experimental procedures seem quite satisfactory however. The following solubility value based entirely upon the work reported by Blackman et al., must be considered as doubtful.

T/K	$10^4 \text{ mol}(1)/\text{dm}^3$	10g(1)/kg	$10^5 x(1)$
298.15	7.9	1.8	1.4

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

COMPONENTS: (1) 2,3,4,6-Tetrachlorophenol; $C_6H_2Cl_4O$; [58-90-2] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Blackman, G. E.; Parke, M. H.; Garton, G. <i>Arch. Biochem. Biophys.</i> <u>1955</u> , <i>54</i> (1), 55-71.								
VARIABLES: One temperature One pH: 5.1	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;">$10g(1)/dm^3$ ^a</th> <th style="text-align: left; padding-right: 20px;">$10^4 mol(1)/dm^3$ ^b</th> <th style="text-align: left;">$10^5 x(1)$ ^a</th> </tr> </thead> <tbody> <tr> <td style="text-align: left; padding-right: 20px;">25</td> <td style="text-align: left; padding-right: 20px;">1.83</td> <td style="text-align: left; padding-right: 20px;">7.9</td> <td style="text-align: left;">1.43</td> </tr> </tbody> </table> <p>a. Calculated by F. W. Getzen b. Reported value measured at pH 5.1.</p>		$t/^{\circ}C$	$10g(1)/dm^3$ ^a	$10^4 mol(1)/dm^3$ ^b	$10^5 x(1)$ ^a	25	1.83	7.9	1.43
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25	1.83	7.9	1.43						
AUXILIARY INFORMATION									
METHOD/APPARATUS/PROCEDURE: The samples were equilibrated in a thermostat bath with intermittent shaking over periods of 3-4 weeks. During the equilibration time, the pH values of the solutions were controlled by dropwise addition of phosphate buffer solution. The analysis of the solute concentration in the saturated samples was done spectrophotometrically either directly or by using proper colorizing agents.	SOURCE AND PURITY OF MATERIALS: $C_6H_2Cl_4O$: Not specified, probably a commercial product. H_2O : Distilled water.								
	ESTIMATED ERROR: Solubility: <5% (estimated here on the basis of the reported results of the two techniques of analysis).								
	REFERENCES:								