

COMPONENTS:

- (1) 2,4,5-Trichlorophenol; $C_6H_3Cl_3O$;
[95-95-4]
- (2) Water; H_2O ; [7732-18-5]

EVALUATOR:

A. Vesala, Department of Chemistry and
Biochemistry, University of Turku.

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CRITICAL EVALUATION:

The solubility 2,4,5-trichlorophenol in aqueous buffer solution has been reported by Blackman, Parke, and Garton (1) in 1954. The principal motivation of this study was to observe the relationships between physical properties and physiological activities of certain substituted phenols. The experimental conditions were standardized with respect to pH by the slight addition of a phosphate buffer to the test solutions. The final pH value of the saturated solutions was regulated to 5.1. Under saturation equilibrium conditions, however, the concentration of the buffer was relatively dilute having a concentration of about 6 mmol/dm^3 relative to the added phosphate, KH_2PO_4 .

The salt effect of the added buffer can be neglected, but the effect of the adjusted pH upon the acid dissociation equilibrium of the phenol must be given some consideration. The acidity constant for the 2,4,5-trichlorophenol was reported by Blackman et al. to have a magnitude in the order of 10^{-7} . Consequently, in the absence of the added buffer, the pH of the saturated solution should fall below the 5.1 value. Therefore, the adjustment of the pH to a value of 5.1 with the buffer should result in an increase in the concentration of the phenoxide ion relative to the undissociated phenol. This situation would result in a higher total solubility compared to the solution without the added buffer.

The authors did undertake tests of their method of analysis. They established the difference between the values measured by what they called "colorimetric" and "spectrophotometric" methods to be approximately 4 percent. However, the information concerning the purity of the reagents used was inadequate. Considering all such factors, the solubility of 2,4,5-trichlorophenol in water must be reported as a doubtful value.

The solubility of 2,4,5-trichlorophenol in water at a pH of 5.1 is reported here as a doubtful value:

T/K	10^3 mol(1)/dm^3	10g(1)/kg	$10^5 x(1)$
298.15	5.0	9.9	9.0

REFERENCES

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

COMPONENTS: (1) 2,4-5-Trichlorophenol; $C_6H_3Cl_3O$; [95-95-4] (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> , 54(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;">$10g(l)/cm^3$ ^a</th> <th style="text-align: left; padding-right: 20px;">$10^3 mol(l)/dm^3$ ^b</th> <th style="text-align: left;">$10^5 x(l)$ ^a</th> </tr> </thead> <tbody> <tr> <td style="text-align: left; padding-right: 20px;">25</td> <td style="text-align: left; padding-right: 20px;">9.48</td> <td style="text-align: left; padding-right: 20px;">4.8</td> <td style="text-align: left;">8.68</td> </tr> </tbody> </table> a. Calculated by F. W. Getzen. b. Reported value measured at pH 5.1.		$t/^\circ C$	$10g(l)/cm^3$ ^a	$10^3 mol(l)/dm^3$ ^b	$10^5 x(l)$ ^a	25	9.48	4.8	8.68
$t/^\circ C$	$10g(l)/cm^3$ ^a	$10^3 mol(l)/dm^3$ ^b	$10^5 x(l)$ ^a						
25	9.48	4.8	8.68						
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: $C_6H_3Cl_3O$: Source and purity not specified, probably a commercial reagent. H_2O : Distilled. ESTIMATED ERROR: Solubility: <5% (evaluated here on the basis of the reported results of the two techniques of analysis). REFERENCES:								