COMPONENTS:	EVALUATOR:
(1) 2,4,5,6-Tetrachloro-3-methylphenol; $C_7H_4Cl_4O$; [10460-33-0] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA July 1983.

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4,5,6-tetrachloro-3-methylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4,5,6-tetrachloro-3-methylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4,5,6-tetrachloro-3-methylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 2,4,5,6-tetrachloro-3-methylphenol in water is tentative:

t/°C	10^3g(1)/dm^3	10^5mol(1)/dm^3	10^7x(1)
25	6.15	2.5	4.52

REFERENCES

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,5,6-Tetrachloro-3-methylphenol; $C_7H_4Cl_4O$; [10460-33-0] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.
VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

t/°C	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	6.15	2.5	4.52

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation.

Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.

SOURCE AND PURITY OF MATERIALS:

$C_7H_4Cl_4O$: Probably a commercial reagent.

H_2O: Distilled water.

ESTIMATED ERROR:

Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).

REFERENCES:

1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, 1936.
2. Folin, O.; Denis, W. *J. Biol. Chem.* 1912, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* 1927, *73*, 627.