| COMPONENTS: | EVALUATOR: |
|---|---|
| (1) 2,4,6-Trichlorophenol; $C_6H_3Cl_3O$; [88-06-2] | A. Vesala, Department of Chemistry and Biochemistry, University of Turku. |
| (2) Water; $H_2O$; [7732-18-5] | November 1979. |

CRITICAL EVALUATION:

Daccomo (1) has provided the first reported measurement of the solubility of 2,4,6-trichlorophenol in water. These measurements were made at least as early as 1885. They can be judged as somewhat unreliable for several reasons. First of all, the melting point of the substrate was 2-3 degrees below that reported later (69.5°C) in the "Handbook of Chemistry and Physics" (2). The measurements themselves were not described. However, it is porbable that the so-called "classical synthetic method" was applied. In this procedure, known amounts of solute and solvent are mixed and their miscibilities tested with temperature. The reported value of 0.85 g(1)/kg(2) at 298 K from three experimental points does not allow one to establish a reliable estimate of experimental errors.

Another value for the solubility of 2,4,6-trichlorophenol in water has been reported by Blackman, Parke, and Garton (3). Their determination was made at a solution pH of 5.1 through the slight addition of a phosphate buffer solution. Because the phenol in question has an acid pK value of 10.9 according to Blackman et al., the buffer solution pH evidently suppresses the ionization. This results in a decrease in concentration of the phenolate ion relative to the undissociated phenol. The net result is that the solubility should be suppressed somewhat for the buffered system relative to that for a system containing only the phenol itself in water. Converting the solubility value to the same units as those of Daccomo (using a solution density of 1.0 g/cm$^3$), one obtains a value of 0.443 g(1)/kg(2) at the pH value of 5.1. This solubility value is quite possible, relative to the value provided by Daccomo, for the reasons indicated.

Since the variation of solubility with pH is not known in this case, only a doubtful value for the solubility of 2,4,6-trichlorophenol in water can be reported here. The value of Daccomo refers to a solution saturated with only the phenol at the pH which prevails for a saturated solution. Therefore, this value has been selected as the most appropriate saturation value at 298.15 K.

The solubility of 2,4,6-trichlorophenol in water is reported here as a doubtful value:

| T/K | $10^3$mol(1)/dm$^3$ | 10g(1)/kg | $10^5x$(1) |
|---|---|---|---|
| 298.15 | 2.2 | 4.3 | 4.0 |

REFERENCES

1. Daccomo, G. *Ber. Dtsch. Chem. Ges.* 1885, *18*, 1163-4.

2. "Handbook of Chemistry and Physics", 50th ed.; Weast, R. C., Ed.; CRC Press: Cleveland, Ohio, 1969; p C-426.

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

| COMPONENTS: | ORIGINAL MEASUREMENTS: |
|---|---|
| (1) 2,4,6-Trichlorophenol; $C_6H_3Cl_3O$; [88-06-2]<br>(2) Water; $H_2O$; [7732-18-5] | Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71. |
| VARIABLES:<br>One temperature<br>One pH: 5.1 | PREPARED BY:<br>A. Vesala |

EXPERIMENTAL VALUES:

| t/°C | $10g(1)/dm^3$ [a] | $10^3 mol(1)/dm^3$ [b] | $10^5 x(1)$ [a] |
|---|---|---|---|
| 25 | 4.34 | 2.2 | 3.98 |

a. Calculated by F. W. Getzen.
b. Reported value measured at pH 5.1.

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:
$C_6H_3Cl_3O$: Not specified, probably a commercial product.

$H_2O$: Distilled.

ESTIMATED ERROR:
Solubility: <5% (evaluated here on the basis of the reported results of the two techniques of analysis).

REFERENCES:

| COMPONENTS: | ORIGINAL MEASUREMENTS: |
|---|---|
| (1) 2,4,6-Trichlorophenol; $C_6H_3Cl_3O$; [88-06-2]<br>(2) Water; $H_2O$; [7732-18-5] | Daccomo, G. *Ber. Dtsch. Chem. Ges.* 1885, *18*, 1163-4. |
| VARIABLES: | PREPARED BY: |
| Temperature | A. Vesala |

EXPERIMENTAL VALUES:

| t/°C | 10g(1)/kg(2) [a] | $10^3$mol(1)/kg [b] | $10^5 x$(1) [b] |
|---|---|---|---|
| 11.2 | 5.10 | 2.581 | 4.653 |
| 25.4 | 8.58 | 4.341 | 7.828 |
| 96 | 24.3 | 12.28 | 22.17 |

a. Reported (parts(1) per 1000 parts(2) in original work).
b. Calculated by F. W. Getzen.

Measurements are shown graphically in Figure 1.

Continued ...

AUXILIARY INFORMATION

| METHOD/APPARATUS/PROCEDURE: | SOURCE AND PURITY OF MATERIALS: |
|---|---|
| No specifications given. Probably the so-called synthetic method. | $C_6H_3Cl_3O$: Synthesized both from 2-chlorophenol and 4-chlorophenol, melting point 67°C.<br>$H_2O$: Source and purity not specified. |
| | ESTIMATED ERROR: |
| | REFERENCES: |

| COMPONENTS: | ORIGINAL MEASUREMENTS: |
|---|---|
| (1) 2,4,6-Trichlorophenol; $C_6H_3Cl_3O$; [88-06-2]<br>(2) Water; $H_2O$; [7732-18-5] | Daccomo, G. *Ber. Dtsch. Chem. Ges.* 1885, *18*, 1163-4. |

EXPERIMENTAL VALUES: Continued ...

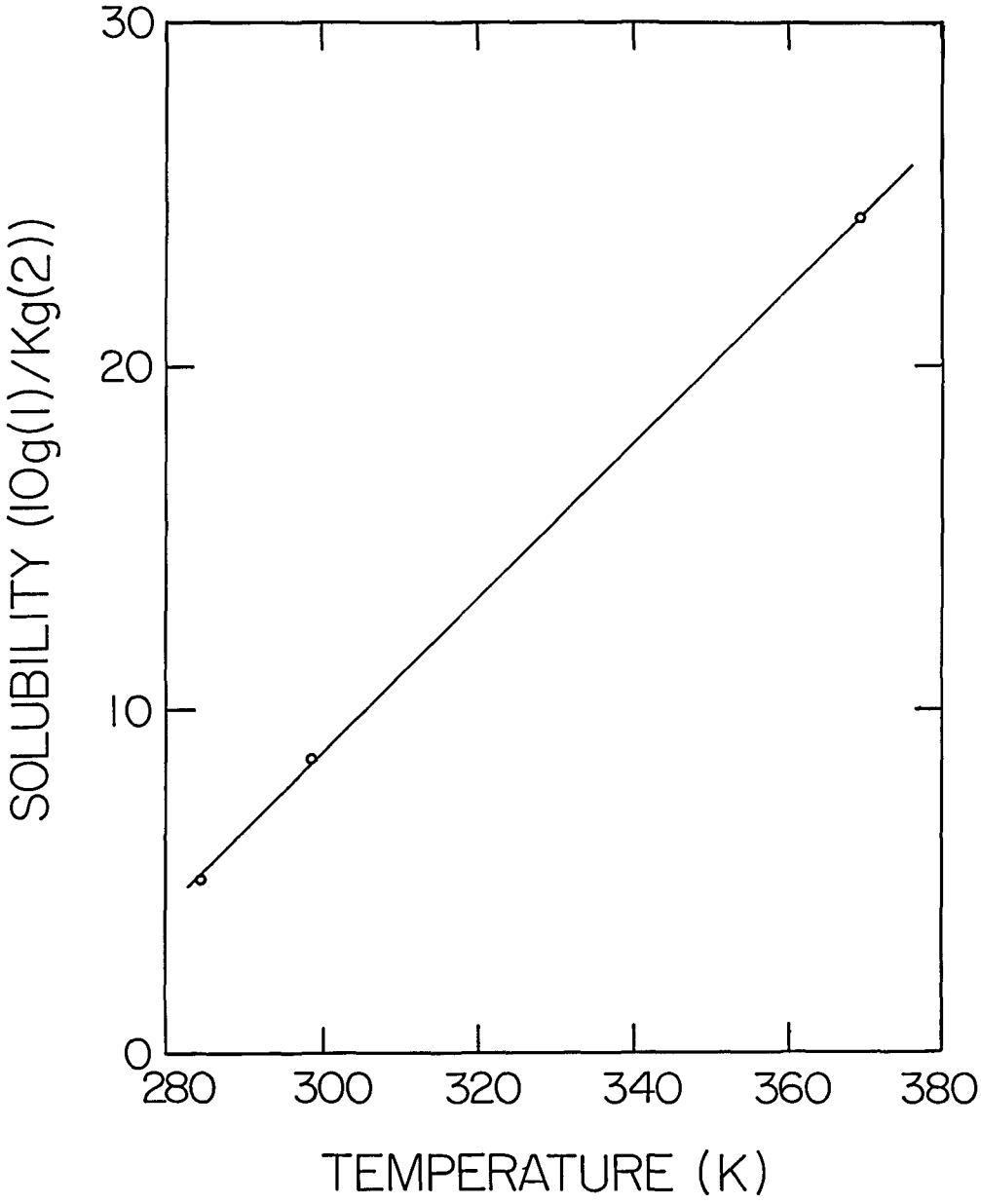


Figure 1. Solubility of 2,4,6-trichlorophenol in water versus Absolute temperature.