

<p>COMPONENTS:</p> <p>(1) Pentachlorophenol; C_6HCl_5O; [87-86-5]</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>
---	--

CRITICAL EVALUATION:

The solubility of pentachlorophenol in water was first reported by Carswell and Nason (1) in 1938 in connection with their study of properties and uses of this compound. The determinations were done very rapidly and the method, the classical "synthetic" one, allowed the solubility measurements to be made at various temperatures. When the reported values are fit by linear regression to the logarithm of solubility versus the reciprocal of Absolute temperature, the following equation results:

$$\log_{10}(S_1(g(l))/kg) = (3.517 \pm 0.239) - (1589 \pm 74)/T \quad [1]$$

The coefficient of correlation for equation [1] is 0.997. The calculated value for the solubility of pentachlorophenol from equation [1] is 0.0154 g(l)/kg at 298.15 K. As is evident, the magnitude of the standard error estimate is in the order of 6-7 percent.

Two other reports on the solubility of pentachlorophenol in water take into account the variation of the solubility with hydrogen ion activity. The earlier work published in 1955 by Blackman, Parke, and Garton (2) reported the pH value at which the solubility was measured. The later study by Toyota and Kuwahara (3) in 1967 provided the variation of solubility with pH in water, in aqueous KCl solutions, and in aqueous NH_4Cl solutions. Also provided in their work was an empirical equation for the solubility in water with respect to pH.

The ability of pentachlorophenol to protolyze in water makes the question of its solubility somewhat complicated. In order to establish the solubility behavior generally, one must measure solubilities with pH as one of the variables. The information provided in (2) and (3) is, however, too limited to allow further calculations in this respect. Thus, in reality, it is practical to evaluate and report only the total solubility of pentachlorophenol/phenoxide at the pH prevailing in the saturated solution. This total solubility can be compared with the value obtained from equation [1].

Some critical observations can be made concerning the measurements of Toyota and Kuwahara. First of all, no description of the sources and purities of reagents was provided. Also, the method of analysis was gravimetric based upon the assumption that the pentachlorophenol was insoluble at pH values lower than 3. That is, the saturation value was established by weighing the pentachlorophenol precipitated from a saturated solution with its pH suppressed below 3. Thus, the method rejected the solubility of pentachlorophenol at pH values lower than 3. Such a method permits the determination of total concentration of saturated solutions only at elevated pH values (from pH 6 and up; pH 5 seems too low). The accuracy of the method is not sufficient to determine the cosolute effects of urea, KCl, and NH_4Cl either. This can be seen clearly from the plots of $\log(s/s_0)$ versus the concentration of the cosolute. The complicated behavior is understandable in view of the fact that the cosolutes may have dissimilar effects on the phenol and the phenoxide ion. Therefore, the values must be discarded and the solubilities in water must be checked against other values available. Blackman et al. reported the total solubility of pentachlorophenol at pH 5.1. This hydrogen ion activity was established by the use of a phosphate buffer in amounts which may have been insufficient to affect the solubility. Therefore, this value can be taken as comparable with the value of Carswell and Nason provided the pH of the solution is taken to be in the range 4.5-5.5.

On the basis of the three solubilities available, 1.4×10^{-2} g(l)/kg from (1), a 9.6×10^{-3} g(l)/kg from (2), and 1.4×10^{-2} g(l)/kg from (3), the following is a tentative solubility value. (The last of these three values was calculated from the equation provided in (3) and it refers to 300 K.) Also, it must be emphasized that, as for any protolyzing solute, the solubility of pentachlorophenol in water is affected to a degree by changes in pH.

T/K	10^5 mol(l)/dm^3	10^2 g(l)/kg	$10^7 x(1)$
298.15	3.7	1.0	6.8

<p>COMPONENTS:</p> <p>(1) Pentachlorophenol; C_6HCl_5O; [87-86-5]</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>
<p>CRITICAL EVALUATION: (Continued)</p> <p style="text-align: center;">REFERENCES</p> <ol style="list-style-type: none">1. Carswell, T. S.; Nason, H. K. <i>Ind. Eng. Chem.</i> <u>1938</u>, <i>30(6)</i>, 622-6.2. Blackman, G. E.; Park, M. H.; Garton, G. <i>Arch. Biochem. Biophys.</i> <u>1955</u>, <i>54(1)</i>, 55-71.3. Toyota, H.; Kuwahara, M. <i>Nippon Dojohiryogaku Zasshi</i> <u>1967</u>, <i>38(2,3)</i>, 93-97.	

COMPONENTS: (1) Pentachlorophenol; C_6HCl_5O ; [87-86-5] (2) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Carswell, T. S.; Nason, H. K. <i>Ind. Eng. Chem.</i> <u>1938</u> , <i>30(6)</i> , 622-6.																								
VARIABLES: Temperature: 0 - 70°C	PREPARED BY: A. Vesala																								
EXPERIMENTAL VALUES: <table border="1" data-bbox="255 483 967 772"> <thead> <tr> <th>$t/^\circ C$</th> <th>$10^2 g(1)/kg^a$</th> <th>$10^5 mol(1)/kg^b$</th> <th>$10^7 x(1)^b$</th> </tr> </thead> <tbody> <tr> <td>0</td> <td>0.5</td> <td>1.9</td> <td>3.4</td> </tr> <tr> <td>27</td> <td>1.8</td> <td>6.76</td> <td>12.2</td> </tr> <tr> <td>50</td> <td>3.5</td> <td>13.1</td> <td>23.7</td> </tr> <tr> <td>62</td> <td>5.8</td> <td>21.8</td> <td>39.2</td> </tr> <tr> <td>70</td> <td>8.5</td> <td>31.9</td> <td>57.5</td> </tr> </tbody> </table> <p data-bbox="255 801 994 859"> a. Reported (values given as percent (1) in original work). b. Calculated by F. W. Getzen. </p> <p data-bbox="255 898 840 927"> Measurements are shown graphically in Figure 1. </p> <p data-bbox="1115 1110 1283 1139" style="text-align: right;">Continued ...</p>		$t/^\circ C$	$10^2 g(1)/kg^a$	$10^5 mol(1)/kg^b$	$10^7 x(1)^b$	0	0.5	1.9	3.4	27	1.8	6.76	12.2	50	3.5	13.1	23.7	62	5.8	21.8	39.2	70	8.5	31.9	57.5
$t/^\circ C$	$10^2 g(1)/kg^a$	$10^5 mol(1)/kg^b$	$10^7 x(1)^b$																						
0	0.5	1.9	3.4																						
27	1.8	6.76	12.2																						
50	3.5	13.1	23.7																						
62	5.8	21.8	39.2																						
70	8.5	31.9	57.5																						
AUXILIARY INFORMATION																									
METHOD/APPARATUS/PROCEDURE: A known amount of pure pentachlorophenol was added to cold water. Then, the temperature was raised slowly with agitation until dissolution was complete.	SOURCE AND PURITY OF MATERIALS: C_5HCl_5O : Source and purity not specified. H_2O : No specifications given.																								
ESTIMATED ERROR: Solubility: <6% (estimated by the evaluator on the basis of the smoothed curve of $\log c$ vs. $1/T$, where c denotes solubility).																									
REFERENCES:																									

COMPONENTS:

- (1) Pentachlorophenol; C_6HCl_5O ; [87-86-5]
(2) Water; H_2O ; [7732-18-5]

ORIGINAL MEASUREMENTS:

Carswell, T. S.; Nason, H. K. *Ind. Eng. Chem.* 1938, 30(6), 622-6.

EXPERIMENTAL VALUES:

Continued ...

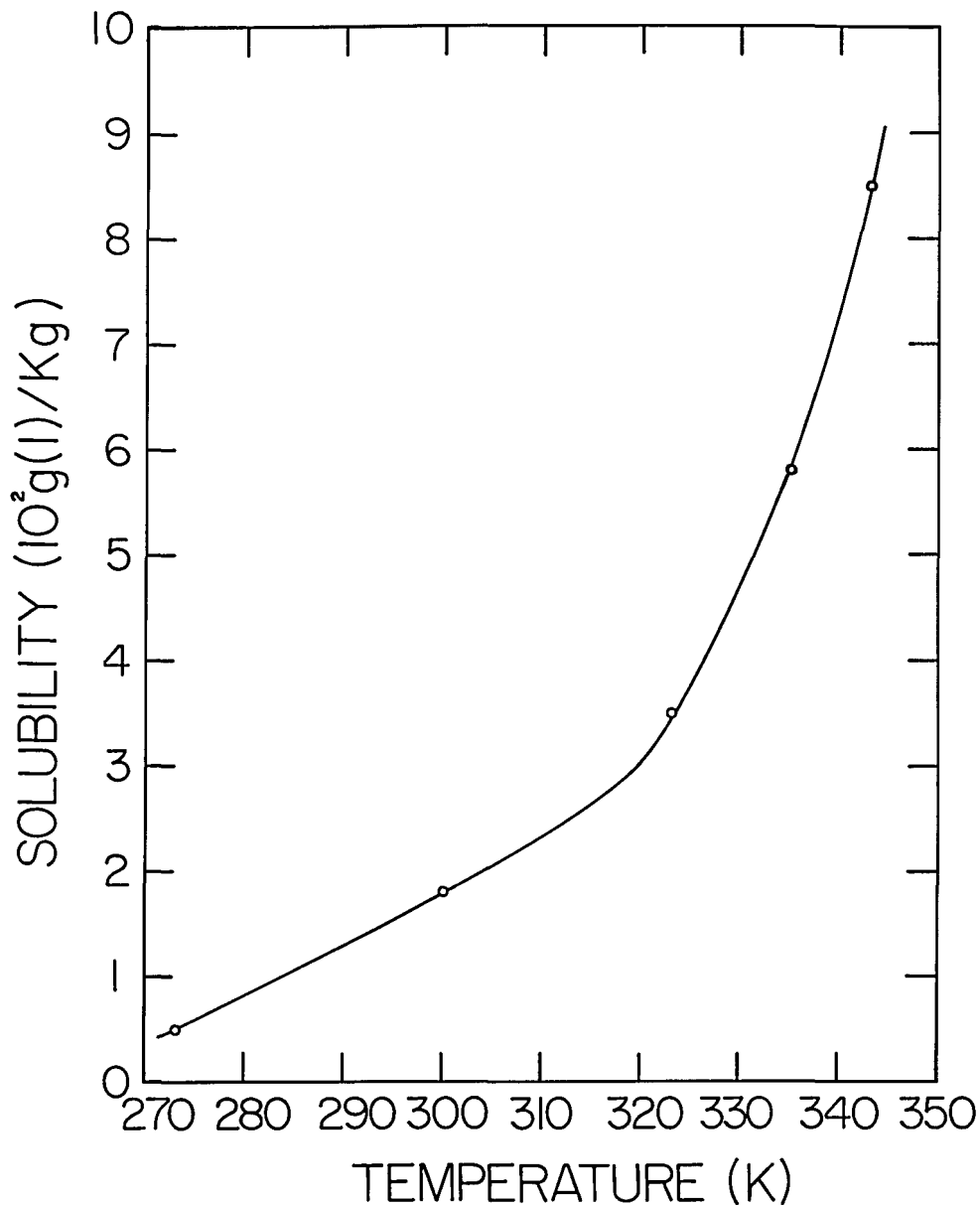


Figure 1. Solubility of pentachlorophenol in water versus Absolute temperature.

<p>COMPONENTS:</p> <p>(1) Pentachlorophenol; C_6HCl_5O; [87-86-5]</p> <p>(2) Water; H_2O; [7732-18-5]</p>	<p>ORIGINAL MEASUREMENTS:</p> <p>Blackman, G. E.; Parke, M. H.; Garton, G. <i>Arch. Biochem. Biophys.</i> <u>1955</u>, <i>54</i>(1), 55-71.</p>								
<p>VARIABLES:</p> <p>One temperature</p> <p>One pH: 5.1</p>	<p>PREPARED BY:</p> <p>A. Vesala</p>								
<p>EXPERIMENTAL VALUES:</p> <table data-bbox="256 479 995 566"> <thead> <tr> <th>$t/^\circ C$</th> <th>$10^3 g(1)/dm^3$ ^a</th> <th>$10^5 mol(1)/dm^3$ ^b</th> <th>$10^7 x(1)$ ^a</th> </tr> </thead> <tbody> <tr> <td>25</td> <td>9.59</td> <td>3.6</td> <td>6.51</td> </tr> </tbody> </table> <p>a. Calculated by F. W. Getzen.</p> <p>b. Reported value measured at pH 5.1.</p>		$t/^\circ C$	$10^3 g(1)/dm^3$ ^a	$10^5 mol(1)/dm^3$ ^b	$10^7 x(1)$ ^a	25	9.59	3.6	6.51
$t/^\circ C$	$10^3 g(1)/dm^3$ ^a	$10^5 mol(1)/dm^3$ ^b	$10^7 x(1)$ ^a						
25	9.59	3.6	6.51						
<p>AUXILIARY INFORMATION</p>									
<p>METHOD/APPARATUS/PROCEDURE:</p> <p>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.</p>	<p>SOURCE AND PURITY OF MATERIALS:</p> <p>C_6HCl_5O: Probably a commercial reagent.</p> <p>H_2O: Distilled water.</p> <p>ESTIMATED ERROR:</p> <p>Solubility: <5% (evaluated on the basis of the reported results of the two techniques of analysis).</p> <p>REFERENCES:</p>								

<p>COMPONENTS:</p> <p>(1) Pentachlorophenol; C_6HCl_5O; [87-86-5]</p> <p>(2) Potassium chloride; KCl; [7447-40-7]</p> <p>(3) Water; H_2O; [7732-18-5]</p>		<p>ORIGINAL MEASUREMENTS:</p> <p>Toyota, H.; Kuwahara, M. <i>Nippon Dojohiryogaku Zasshi</i> 1967, 38(2,3), 93-97.</p>		
<p>VARIABLES:</p> <p>pH, concentrations of KCl at 27°C</p>		<p>PREPARED BY:</p> <p>H. Ohtaki</p>		
<p>EXPERIMENTAL VALUES: All Measurements at 27°C</p>				
<p style="text-align: center;">Initial pH = 5.0</p>				
mol(KCl)/dm ³	10 ² g(1)/dm ³ a	10 ⁵ mol(1)/dm ³ b	10 ⁶ x(1) a,c	pH d
1.0	1.68	6.3	1.13	5.32
0.50	2.32	8.7	1.56	5.45
0.20	1.65	6.2	1.12	5.25
0.10	2.08	7.8	1.41	5.34
0.05	3.20	12	2.17	5.28
0.02	2.16	8.1	1.46	5.20
0.0	3.20	12	2.17	5.35
<p style="text-align: center;">Initial pH = 6.0</p>				
mol(KCl)/dm ³	10g(1)/dm ³ a	10 ⁴ mol(1)/dm ³ b	10 ⁶ x(1) a,c	pH d
1.0	1.01	3.8	6.81	5.96
0.50	0.879	3.3	5.93	5.89
0.20	0.985	3.7	6.67	6.07
Continued				
AUXILIARY INFORMATION				
<p>METHOD/APPARATUS/PROCEDURE:</p> <p>Pentachlorophenol and various amounts of NaOH and KCl were dissolved in water at 27°C and the solutions were left for 3 days with occasional stirring (once a day for 1 hour). Then, the undissolved pentachlorophenol was filtered off and the pH values of the filtrates were measured with a glass electrode. To each aliquot of the solutions was added hydrochloric acid to maintain their pH less than 3. The precipitates which resulted were aged and weighed.</p>		<p>SOURCE AND PURITY OF MATERIALS:</p> <p>Nothing specified.</p>		
		<p>ESTIMATED ERROR: No estimation was given for errors in the solubility measurements. However, the reported values of S/S° (S the solubility of pentachlorophenol in KCl solutions and S° its solubility in pure water) do not fall on a single smooth curve, but rather spread. Therefore, the errors may be estimated to be larger than 2-3%.</p>		
		<p>REFERENCES:</p> <p>1. Nose, K.; Fukunaga, K. <i>Noyaku Seisan Gijutsu</i> 1952, 6, 30.</p>		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
(1) Pentachlorophenol; C_6HCl_5O ; [87-86-5]		Toyota, H.; Kuwahara, M. <i>Nippon Dojohiryogaku Zasshi</i> 1967, 38(2,3), 93-97.		
(2) Potassium chloride; KCl; [7447-40-7]				
(3) Water; H_2O ; [7732-18-5]				
EXPERIMENTAL VALUES: Continued				
Initial pH = 6.0				
mol(KCl)/dm ³	10g(l)/dm ³ a	10 ⁴ mol(l)/dm ³ b	10 ⁶ x(1) a,c	pH d
0.10	1.17	4.4	7.94	6.00
0.05	1.39	5.2	9.38	5.95
0.02	1.54	5.8	10.5	5.98
0.0	0.613	2.3	4.15	5.70
Initial pH = 7.0				
mol(KCl)/dm ³	g(l)/dm ³ a	10 ³ mol(l)/dm ³ b	10 ⁵ x(1) a,c	pH d
1.0	1.01	3.8	6.81	6.81
0.50	1.07	4.0	7.20	6.79
0.20	1.41	5.3	9.56	6.82
0.10	1.25	4.7	8.49	6.77
0.05	1.46	5.5	9.94	6.86
0.02	1.33	5.0	9.03	8.82
0.0	2.05	7.7	13.9	6.92
Initial pH = 8.0				
mol(KCl)/dm ³	10 ⁻¹ g(l)/dm ³ a	10 ² mol(l)/dm ³ b	10 ³ x(1) a,c	pH d
1.0	1.68	6.3	1.15	7.78
0.50	1.57	5.9	1.08	7.67
0.20	2.18	8.2	1.51	7.93
0.10	1.68	6.3	1.15	7.70
0.05	2.45	9.2	1.70	8.35
0.02	1.92	7.2	1.32	7.67
0.0	1.94	7.3	1.34	7.80
a. Calculated by F. W. Getzen.				
b. Reported.				
c. Calculated mole fraction based upon complete dissociation of KCl.				
d. pH value of solution equilibrated with precipitate.				
COMMENTS AND/OR ADDITIONAL DATA:				
Solubilities of pentachlorophenol in water versus hydrogen ion activity, in the absence of KCl, at 27°C were measured and calculated. The stoichiometric amounts of dissolved pentachlorophenol were calculated from mass balance based upon incomplete dissociation. The dissociation constant was given as $K_p = [C_6Cl_5O^-][H^+]/[C_6Cl_5OH] = 3.2 \times 10^{-5} \text{ mol/dm}^3$. This value together with the activity of the hydrogen ion, $\{H^+\}$, as determined from pH measurements was incorporated in an equation for calculating the solubility:				
$s = \frac{1.796 \times 10^{-6}}{\{H^+\}0.170} \left[1 + \frac{3.2 \times 10^{-5}}{\{H^+\}} \right]$				
Observed and calculated values reported:				
pH	5.0	6.0	7.0	
	10 ⁵ mol(l)/dm ³	10 ⁴ mol(l)/dm ³	10 ³ mol(l)/dm ³	
Observed value:	4.05	6.05	8.85	
Calculate value:	5.34	6.20	8.90	

COMPONENTS: (1) Pentachlorophenol; C_6HCl_5O ; [87-86-5] (2) Ammonium chloride; NH_4Cl ; [12125-02-9] (3) Water; H_2O ; [7732-18-5]	ORIGINAL MEASUREMENTS: Toyota, H.; Kuwahara, M. <i>Nippon Dojohiryogaku Zasshi</i> <u>1967</u> , <i>38</i> (2,3), 93-97.																																																																																
VARIABLES: pH, concentrations of NH_4Cl at 27°C	PREPARED BY: H. Ohtaki																																																																																
EXPERIMENTAL VALUES: <p style="text-align: center;">All Measurements at 27°C</p> <table border="0" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th colspan="5" style="text-align: center;">Initial pH = 5.0</th> </tr> <tr> <th style="text-align: left;">$mol(NH_4Cl)/dm^3$</th> <th style="text-align: left;">$10^2 g(l)/dm^3$ ^a</th> <th style="text-align: left;">$10^5 mol(l)/dm^3$ ^b</th> <th style="text-align: left;">$10^7 x(l)$ ^{a,c}</th> <th style="text-align: left;">pH ^d</th> </tr> </thead> <tbody> <tr><td>1.0</td><td>0.8390</td><td>3.15</td><td>5.690</td><td>5.12</td></tr> <tr><td>0.50</td><td>1.377</td><td>5.17</td><td>9.335</td><td>5.20</td></tr> <tr><td>0.05</td><td>3.3161</td><td>12.45</td><td>22.472</td><td>5.41</td></tr> <tr><td>0.0</td><td>3.0657</td><td>11.51</td><td>20.774</td><td>5.35</td></tr> </tbody> </table> <table border="0" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th colspan="5" style="text-align: center;">Initial pH = 5.5</th> </tr> <tr> <th style="text-align: left;">$mol(NH_4Cl)/dm^3$</th> <th style="text-align: left;">$10^2 g(l)/dm^3$ ^a</th> <th style="text-align: left;">$10^4 mol(l)/dm^3$ ^b</th> <th style="text-align: left;">$10^6 x(l)$ ^{a,c}</th> <th style="text-align: left;">pH ^d</th> </tr> </thead> <tbody> <tr><td>0.05</td><td>6.153</td><td>2.31</td><td>4.170</td><td>5.73</td></tr> </tbody> </table> <table border="0" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th colspan="5" style="text-align: center;">Initial pH = 6.0</th> </tr> <tr> <th style="text-align: left;">$mol(NH_4Cl)/dm^3$</th> <th style="text-align: left;">$10g(l)/dm^3$ ^a</th> <th style="text-align: left;">$10^4 mol(l)/dm^3$ ^b</th> <th style="text-align: left;">$10^5 x(l)$ ^{a,c}</th> <th style="text-align: left;">pH ^d</th> </tr> </thead> <tbody> <tr><td>1.0</td><td>1.489</td><td>5.59</td><td>1.010</td><td>6.01</td></tr> <tr><td>0.50</td><td>1.345</td><td>5.05</td><td>0.9120</td><td>6.05</td></tr> <tr><td>0.30</td><td>2.9645</td><td>11.13</td><td>2.0099</td><td>6.19</td></tr> <tr><td>0.20</td><td>2.650</td><td>9.95</td><td>1.797</td><td>6.14</td></tr> <tr><td>0.0</td><td>0.5993</td><td>2.25</td><td>0.4061</td><td>5.70</td></tr> </tbody> </table> <p style="text-align: right;">Continued</p>		Initial pH = 5.0					$mol(NH_4Cl)/dm^3$	$10^2 g(l)/dm^3$ ^a	$10^5 mol(l)/dm^3$ ^b	$10^7 x(l)$ ^{a,c}	pH ^d	1.0	0.8390	3.15	5.690	5.12	0.50	1.377	5.17	9.335	5.20	0.05	3.3161	12.45	22.472	5.41	0.0	3.0657	11.51	20.774	5.35	Initial pH = 5.5					$mol(NH_4Cl)/dm^3$	$10^2 g(l)/dm^3$ ^a	$10^4 mol(l)/dm^3$ ^b	$10^6 x(l)$ ^{a,c}	pH ^d	0.05	6.153	2.31	4.170	5.73	Initial pH = 6.0					$mol(NH_4Cl)/dm^3$	$10g(l)/dm^3$ ^a	$10^4 mol(l)/dm^3$ ^b	$10^5 x(l)$ ^{a,c}	pH ^d	1.0	1.489	5.59	1.010	6.01	0.50	1.345	5.05	0.9120	6.05	0.30	2.9645	11.13	2.0099	6.19	0.20	2.650	9.95	1.797	6.14	0.0	0.5993	2.25	0.4061	5.70
Initial pH = 5.0																																																																																	
$mol(NH_4Cl)/dm^3$	$10^2 g(l)/dm^3$ ^a	$10^5 mol(l)/dm^3$ ^b	$10^7 x(l)$ ^{a,c}	pH ^d																																																																													
1.0	0.8390	3.15	5.690	5.12																																																																													
0.50	1.377	5.17	9.335	5.20																																																																													
0.05	3.3161	12.45	22.472	5.41																																																																													
0.0	3.0657	11.51	20.774	5.35																																																																													
Initial pH = 5.5																																																																																	
$mol(NH_4Cl)/dm^3$	$10^2 g(l)/dm^3$ ^a	$10^4 mol(l)/dm^3$ ^b	$10^6 x(l)$ ^{a,c}	pH ^d																																																																													
0.05	6.153	2.31	4.170	5.73																																																																													
Initial pH = 6.0																																																																																	
$mol(NH_4Cl)/dm^3$	$10g(l)/dm^3$ ^a	$10^4 mol(l)/dm^3$ ^b	$10^5 x(l)$ ^{a,c}	pH ^d																																																																													
1.0	1.489	5.59	1.010	6.01																																																																													
0.50	1.345	5.05	0.9120	6.05																																																																													
0.30	2.9645	11.13	2.0099	6.19																																																																													
0.20	2.650	9.95	1.797	6.14																																																																													
0.0	0.5993	2.25	0.4061	5.70																																																																													
AUXILIARY INFORMATION																																																																																	
METHOD/APPARATUS/PROCEDURE: Pentachlorophenol and various amounts of NaOH and NH_4Cl were dissolved in water at 27°C and the solutions were left for 3 days with occasional stirring (once a day for 1 hour). Then, the undissolved pentachlorophenol was filtered off and the pH values of the filtrates were measured with a glass electrode. To each aliquot of the solutions was added hydrochloric acid to maintain their pH less than 3. The precipitates which resulted were aged and weighed.	SOURCE AND PURITY OF MATERIALS: Nothing specified.																																																																																
ESTIMATED ERROR: No estimation was given for errors in the solubility measurements. However, the reported values of S/S° (S the solubility of pentachlorophenol in KCl solutions and S° its solubility in pure water) do not fall on a single smooth curve, but rather spread. Therefore, the errors may be estimated to be larger than 2-3%.																																																																																	
REFERENCES:																																																																																	

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorophenol; C_6HCl_5O ; [87-86-5]	Toyota, H.; Kuwahara, M. <i>Nippon Dojohiryogaku Zasshi</i> <u>1967</u> , 38(2,3), 93-97.
(2) Ammonium chloride; NH_4Cl ; [12125-02-9]	
(2) Water; H_2O ; [7732-18-5]	

EXPERIMENTAL VALUES: Continued

Initial pH = 6.5				
$mol(NH_4Cl)/dm^3$	$10g(l)/dm^3$ ^a	$10^3 mol(l)/dm^3$ ^b	$10^5 x(1)$ ^{a,c}	pH ^d
1.0	2.352	0.883	1.595	6.46
0.50	3.9819	1.495	2.7005	6.50
0.10	5.966	2.24	4.045	6.40
0.0	6.233	2.34	4.226	6.52

Initial pH = 7.0				
$mol(NH_4Cl)/dm^3$	$10g(l)/dm^3$ ^a	$10^3 mol(l)/dm^3$ ^b	$10^5 x(1)$ ^{a,c}	pH ^d
1.0	2.9432	1.105	1.9967	6.97
0.50	5.114	1.92	3.469	6.98
0.30	7.777	2.92	5.275	7.03
0.20	8.736	3.28	5.926	7.10
0.10	11.13	4.18	7.553	6.86
0.05	14.76	5.54	10.01	6.92
0.0	20.40	7.66	13.85	6.92

Initial pH = 7.5				
$mol(NH_4Cl)/dm^3$	$g(l)/dm^3$ ^a	$10^3 mol(l)/dm^3$ ^b	$10^4 x(1)$ ^{a,c}	pH ^d
0.10	1.675	6.29	1.137	7.50

Initial pH = 8.0				
$mol(NH_4Cl)/dm^3$	$g(l)/dm^3$ ^a	$10^3 mol(l)/dm^3$ ^b	$10^5 x(1)$ ^{a,c}	pH ^d
1.0	0.3276	1.23	2.223	8.02
0.50	0.5780	2.17	3.920	8.00
0.30	0.6339	2.38	4.299	8.05
0.20	1.247	4.68	8.458	8.01
0.10	1.851	6.95	12.57	8.01
0.05	2.903	10.9	19.73	7.98
0.0	19.39	72.8	133.8	7.80

a. Calculated by F. W. Getzen.

b. Reported.

c. Calculated mole fraction based upon complete dissociation of NH_4Cl .

d. pH value of solution equilibrated with precipitate.

COMMENTS AND/OR ADDITIONAL DATA:

Solubilities of pentachlorophenol in water versus hydrogen ion activity, in the absence of NH_4Cl , at 27°C were measured and calculated. The stoichiometric amounts of dissolved pentachlorophenol were calculated from mass balance based upon incomplete dissociation. The dissociation constant was given as $K_p = [C_6Cl_5O^-][H^+]/[C_6Cl_5OH] = 3.2 \times 10^{-5} mol/dm^3$. This value together with the activity of the hydrogen ion, $\{H^+\}$, as determined from pH measurements was incorporated in an equation for calculating the solubility:

$$s = \frac{1.796 \times 10^{-6}}{\{H^+\}^{0.170}} \left[1 + \frac{3.2 \times 10^{-5}}{\{H^+\}} \right]$$

Observed and calculated values reported:

pH	5.0	6.0	7.0
	$10^5 mol(l)/dm^3$	$10^4 mol(l)/dm^3$	$10^3 mol(l)/dm^3$
Observed value:	4.05	6.05	8.85
Calculate value:	5.34	6.20	8.90