the functions $y_{b+c,m}$, $y_{b+c,m+1}$, ..., $y_{b+c,2m+1}$; thus, the convolution can be expressed in closed form but it may not be compact enough for easy use.

**Representation of X-ray peaks**

Fig. 1 shows two well determined and nearly symmetric X-ray peaks plotted as points obtained by step counting. The continuous curves in (a) and (b) are Pearson type VII $m = 3$ distributions fitted for $y_0$, $\bar{x}$, and $a$ by a standard nonlinear regression analysis. The fit appears to be satisfactory for both the broad and the narrow peaks. Table 2 shows the variation of the fit with variation in $m$. Fig. 2 shows a highly asymmetric peak which was determined similarly. This peak was hypothesized to be a sum of two peaks. Each was characterized by a Pearson type VII distribution with $m = 3$ and the same nonlinear regression program adjusted $y_0$, $\bar{x}$, and $a$ values for both peaks. The resulting curve is shown as the continuous line in Fig. 2. The fit is characterized as in Table 2 by a r.m.s. deviation of 3.37%. The three parameters of the component curves were found in this investigation to be interesting and smoothly varying experimental parameters.

**Conclusions**

Pearson type VII distributions appear to approximate the shape of some symmetric X-ray diffraction peaks. This distribution is Cauchy at $m = 1$, modified Lorentzian at $m = 2$, and Gaussian at $m = \infty$. Its use is illustrated.

This work is supported by the National Science Foundation under Grant GH 40440.

**Table 2. Fitting a broad and a narrow X-ray peak**

<table>
<thead>
<tr>
<th>$m$</th>
<th>Name</th>
<th>Narrow Fig. 1(a)</th>
<th>Broad Fig. 1(b)</th>
</tr>
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<tbody>
<tr>
<td>1</td>
<td>Cauchy</td>
<td>11.80</td>
<td>15.96</td>
</tr>
<tr>
<td>2</td>
<td>Modified Lorentz</td>
<td>3.28</td>
<td>6.11</td>
</tr>
<tr>
<td>2-49</td>
<td>Optimum $m$</td>
<td>2.75</td>
<td>6.51</td>
</tr>
<tr>
<td>3</td>
<td>Fig. 1</td>
<td>3.01</td>
<td>3.30</td>
</tr>
<tr>
<td>4.09</td>
<td>Optimum $m$</td>
<td>3.01</td>
<td>3.30</td>
</tr>
<tr>
<td>$\infty$</td>
<td>Gauss</td>
<td>7.25</td>
<td>5.80</td>
</tr>
</tbody>
</table>

References


**J. Appl. Cryst.** (1977). 10, 68

The problem of white radiation in the measurement of intensities with a solid-state detector: erratum.


(Received 29 November 1976)

In Howard & Jones [J. Appl. Cryst. (1976), 9, 235] the first author's initials should be C.J. and not H.J.

All information is given in the abstract.

**Crystal Data**


Crystal data for some molecular complexes of hexamethylenetetramine with phenols. By Chi-sang Tse, Yau-shing Wong and Thomas C. W. Mak,* Department of Chemistry, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong

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Crystal data are reported for molecular compounds of hexamethylenetetramine with phenol (1:1), resorcinol (1:1), hydroquinone (1:1), o-cresol (1:1), m-cresol (1:2), p-chlorophenol (1:2), and p-bromophenol (1:2).

Hexamethylenetetramine forms molecular complexes with phenol in molar ratios 1:3 (Moschatos & Tollens, 1892) and 1:1 (Smith & Welch, 1934). The crystal structure of the 1:3 adduct has been reported (Jordan & Mak, 1970). In the present study we present crystal data for the 1:1 adduct and six other molecular complexes of hexamethylenetetramine with substituted phenols (Altpeter, 1931).

**Origin of specimens**

Each adduct was prepared by mixing saturated solutions of its two components in stoichiometric proportions and...
heating the resulting solution in a water bath for 15-30 min.
Aqueous ethanol was used as the solvent for all compounds except the 1:1 phenol adduct, for which absolute ethanol was essential. Generally a good crop of crystals was obtained by slow evaporation of the cooled solution under an atmosphere of nitrogen. The crystal data were obtained from Weissenberg photographs taken with Ni-filtered Cu Kα radiation and calibrated with superimposed NaCl powder lines. The densities were measured by flotation in a n-hexane/carbon tetrachloride mixture.

Crystal data

**Hexamethylenetetramine-phenol 1:1,** (CH₂)₆N₄. C₆H₆OH
Colourless elongated prisms, melting point 176°C, slowly crumbles into powder upon exposure to air. C₁₂H₁₈O₃N₄, M₉ = 234.30. Orthorhombic, a = 10.11 (1), b = 7.17 (1), c = 16.80 (2) Å, V = 1218 Å³, Dₚ = 1.280 (5), Dₓ(Z=4) = 1.278 g cm⁻³. Space group C2cm, Cmc2₁, or Cmcm. μ = 6.9 cm⁻¹ (λ = 1.5418 Å).

**Hexamethylenetetramine-resorcinol 1:1,** (CH₂)₆N₄. m-C₆H₄(OH)₂
Colourless elongated prisms, melting point 158-159°C. C₁₂H₁₈O₃N₄, M₉ = 250.30. Orthorhombic, a = 10.40 (1), b = 7.120 (5), c = 16.88 (1) Å, V = 1250 Å³, Dₚ = 1.333 (5), Dₓ(Z=4) = 1.331 g cm⁻³. Space group C2cm, Cmc2₁, or Cmcm. μ = 7.76 cm⁻¹ (λ = 1.5418 Å).

**Hexamethylenetetramine-hydroquinone 1:1,** (CH₂)₆N₄. p-C₆H₄(OH)₂
Colourless prisms, melting point 201-202°C. C₁₂H₁₈O₃N₄, M₉ = 250-30. Monoclinic, a = 6.056 (5), b = 16.70 (1), c = 6.627 (5) Å, β = 110.8 (1)°, V = 626.5 Å³, Dₚ = 1.334 (5), Dₓ(Z=2) = 1.327 g cm⁻³. Space group P2₁ or P2₁/m. μ = 6.64 cm⁻¹ (λ = 1.5418 Å).

**Hexamethylenetetramine-o-cresol 1:1,** (CH₂)₆N₄. o-CH₃C₆H₄OH
Colourless elongated prisms, melting point 98°C, slowly crumbles into powder over a period of several days. C₁₂H₁₈O₃N₄, M₉ = 248.33. Orthorhombic, a = 21.05 (2), b = 17.45 (1), c = 7.26 (1) Å, V = 2667 Å³, Dₚ = 1.244 (5), Dₓ(Z=8) = 1.237 g cm⁻³. Space group Pccn. μ = 6.64 cm⁻¹ (λ = 1.5418 Å).

**Hexamethylenetetramine-m-cresol 1:2,** (CH₂)₆N₄. 2m-CH₃C₆H₄OH
Colourless elongated prisms, melting point 88°C, slowly crumbles into powder upon standing in air. C₂₀H₂₄O₂N₄, M₉ = 356.47. Orthorhombic, a = 10.62 (1), b = 26.35 (2), c = 7.20 (1) Å, V = 2015 Å³, Dₚ = 1.189 (5), Dₓ(Z=4) = 1.175 g cm⁻³. Space group Ccc2 or Ccmm. μ = 6.29 cm⁻¹ (λ = 1.5418 Å).

**Hexamethylenetetramine-p-chlorophenol 1:2,** (CH₂)₆N₄.2p-C₁₂C₆H₄OH
Colourless needles, melting point 97°C, slowly crumbles into powder upon standing in air. C₁₈H₁₂O₂N₄Cl₂, M₉ = 397.31. Monoclinic, a = 16.32 (1), b = 5.850 (5), c = 20.76 (2) Å, β = 94.20 (5)°, V = 1977 Å³, Dₚ = 1.337, Dₓ(Z=4) = 1.335 g cm⁻³. Space group P2₁/c. μ = 31.3 cm⁻¹ (λ = 1.5418 Å).

**Hexamethylenetetramine-p-bromophenol 1:2,** (CH₂)₆N₄.2p-BrC₆H₄OH
Colourless needles, melting point 101°C, slowly crumbles into powder upon standing in air. C₁₈H₁₂O₂N₄Br₂, M₉ = 486.22. Monoclinic, a = 16.46 (1), b = 5.960 (5), c = 21.15 (1) Å, β = 93.94 (5)°, V = 2070 Å³, Dₚ = 1.564, Dₓ(Z=4) = 1.560 g cm⁻³. Space group P2₁/c. μ = 56.9 cm⁻¹ (λ = 1.5418 Å).

Discussion

All the compounds studied have unknown crystal structures. The p-chlorophenol and p-bromophenol adducts are isostructural as one would normally expect. It is however rather surprising that the resorcinol and phenol adducts should turn out to be isostructural. The fact that the former is stable and the latter is not can be rationalized on the grounds that resorcinol is capable of forming twice as many hydrogen bonds as phenol in the crystal lattice. It is noteworthy that all 1:2 adducts examined are relatively unstable and that hydroquinone, which shows a marked tendency to form quinol clathrates (Palin & Powell, 1948) and other hydrogen-bonded molecular crystals (Lee & Wallwork, 1958; Mahmoud & Wallwork, 1975), gives rise to the most stable adduct with hexamethylenetetramine.

References


