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## Crystallographic data for two sugar-alcohols.

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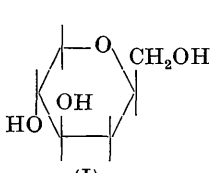
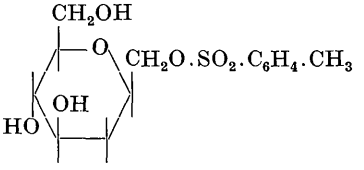
The two compounds were investigated to determine the configurations of hexitols and heptitols obtained by hydroformylation of glucals and arabinals (Rosenthal & Read, 1963). The crystal data were determined from various rotation, Weissenberg, and precession photographs.




(I)




(II)

*Crystal data*

($\lambda$(Cu $K\alpha$) = 1·5418 Å; $\lambda$(Mo $K\alpha$) = 0·7107 Å).

1,5-Anhydro-4-deoxy-D-*arabo*-hexitol (I), $C_6H_{12}O_4$, M.W. 148·2.

Orthorhombic,

$a = 11{\cdot}47 \pm 0{\cdot}01$, $b = 8{\cdot}14 \pm 0{\cdot}01$, $c = 7{\cdot}52 \pm 0{\cdot}01$ Å.

$U = 702$ Å$^3$.

$D_m = 1{\cdot}4$, $Z = 4$, $D_x = 1{\cdot}40$ g.cm$^{-3}$.

Absent spectra: $h00$ when $h$ is odd, $0k0$ when $k$ is odd, $00l$ when $l$ is odd. Space group is $P2_12_12_1$.

1-*O*-(*p*-Toluenesulphonyl)-2,6-anhydro-3-deoxy-D-*gluco*-heptitol (II), $C_{14}H_{20}O_7S$, M.W. 332·3.

Monoclinic,

$a = 8{\cdot}52 \pm 0{\cdot}01$, $b = 33{\cdot}81 \pm 0{\cdot}05$, $c = 6{\cdot}25 \pm 0{\cdot}01$ Å;
$\beta = 116{\cdot}3 \pm 0{\cdot}1°$.

$U = 1614$ Å$^3$.

$D_m = 1{\cdot}33$, $Z = 4$, $D_x = 1{\cdot}37$ g.cm$^{-3}$.

Absent spectra: $0k0$ when $k$ is odd. Space group is $P2_1$.

A more suitable derivative was obtained (Camerman & Trotter, 1964), and no further detailed analysis is planned.

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## The representation of absorption correction factors for spherical and cylindrical crystals by Gaussian functions.

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A correction of the observed intensities of diffracted X-ray or neutron beams for specimen absorption is most conveniently applied when the crystal is of spherical or cylindrical shape. The relevant correction factors for these two cases are tabulated in Tables 5·3·5B and 5·3·6B of *International Tables for X-ray Crystallography* (1959). There, for each value of $\mu R$ in the interval 0–(0·1)–10·0 the correction factors are given for $\theta = 0°$–(5°)–90°.

For a combined computation of the Lorentz, polarization, and specimen absorption correction it would seem desirable to have the data of the above-mentioned tables available in the form of a continuous function rather than as tables, which require many-point interpolation. Furthermore such a function should preferably be expressed in $\sin^2\theta$ (or $\sin^2\Upsilon/2$ for the equi-inclination technique and a cylindrical specimen) rather than in $\theta$, as the computation of $\sin^2\theta$ from the lattice constants is a prerequisite for the Lorentz-polarization correction.

We have found that in the most desirable range of $\mu R$ ($\mu R < 3$) $A^*$ (the absorption correction factor) can be expressed by a simple three-constant formula of the following nature:

$$A^* = a \exp(-b \sin^2\theta) + (A^*_{\theta=0} - a) \exp(-c \sin^2\theta). \quad (1)$$

This function has first been proposed by Vand, Eiland & Pepinsky (1957) for the representation of atomic scattering factors.

In formula (1) $A^*_{\theta=0}$ is the value of $A^*$ in the direction of the primary beam (the first entry in Tables 5·3·5B and 5·3·6B), while $a$, $b$ and $c$ are the three constants for the particular value of $\mu R$.

We have subjected the data of Tables 5·3·5B and 5·3·6B of *International Tables* to a least-squares procedure in order to evaluate the constants $a$, $b$ and $c$ that give a 'best fit' to the data. The weight assigned to each entry in the Tables was $1/A^*$, in order to ensure a generally constant percentage discrepancy between the 'observed' data and those computed with the help of formula (1).

Our machine computation started with $A^*_{\theta=0}/2$ as