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Crystallographic data for two sugar-alcohols.

By A. CAMERMAN and J. TROTTER. *Department of Chemistry, University of British Columbia, Vancouver 8, B.C., Canada*

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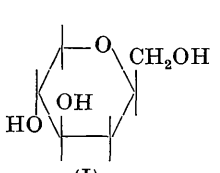
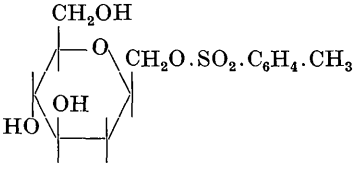
The two compounds were investigated to determine the configurations of hexitols and heptitols obtained by hydroformylation of glucals and arabinals (Rosenthal & Read, 1963). The crystal data were determined from various rotation, Weissenberg, and precession photographs.



(I)



(II)

Crystal data

(λ(Cu $K\alpha$) = 1·5418 Å; λ(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.

The authors are indebted to Dr A. Rosenthal, Mr D. Abson, and Mr H. J. Koch for crystal samples and helpful discussion, and to the National Research Council of Canada for financial support.

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

By J. H. PALM, *Laboratorium voor Technische Natuurkunde der Technische Hogeschool, Lorentzweg* 1, *Delft, The Netherlands*

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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 μR 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 θ, 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 μR ($\mu R < 3$) 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 μR.

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

starting value of a, and the average slope of the high- and low-angle part of the curve through the tabulated data as starting values of b and c, respectively.

Starting from these, a least-squares refinement converged in about five cycles to the final values, except in the cases of the smallest values of μR, where the curve is essentially a straight line. Progress of the refinement of the constants was followed by inspection of the constants and the r.m.s. relative discrepancy between observed and calculated values of μR after every cycle. As a final safeguard $(A^*_{obs}-A^*_{calc})/A^*_{obs}$ was checked for all data in the Tables. In no case did this quantity exceed 1%, so that even in the most unfavourable cases (those with high μR) the structure factors computed with the use of our constants will not be in error by more than 0·5%, and usually by considerably less than that. It should be noted that the original data in the tables are in some places only accurate to within 0·5% owing to round-off.

Table 1. *Analytical constants for the absorption correction factor for spherical crystals*

μR	$A^*_{\theta=0}$	a	b	c	r.m.s. dev.
0·0	1·00	1·000	0·0000	0·0000	0·0%
0·1	1·16	1·160	0·0000	0·0000	0·0
0·2	1·35	1·426	0·0361	0·5831	0·3
0·3	1·56	1·625	0·0581	0·6316	0·1
0·4	1·80	1·820	0·0650	2·3688	0·3
0·5	2·08	2·115	0·1053	0·6462	0·5
0·6	2·39	2·427	0·1395	1·4448	0·2
0·7	2·75	2·812	0·1954	4·2075	0·4
0·8	3·15	3·157	0·2159	4·6021	0·1
0·9	3·61	3·595	0·2592	6·1161	0·1
1·0	4·12	4·058	0·2984	3·0039	0·1
1·1	4·70	4·508	0·3304	2·7231	0·1
1·2	5·35	5·021	0·3670	2·9234	0·1
1·3	6·08	5·671	0·4191	3·7131	0·1
1·4	6·90	6·253	0·4531	3·7853	0·1
1·5	7·80	6·872	0·4869	3·8224	0·1
1·6	8·81	7·620	0·5317	4·2486	0·1
1·7	9·92	8·314	0·5646	4·3171	0·1
1·8	11·2	9·219	0·6145	4·9735	0·2
1·9	12·5	9·839	0·6310	4·5913	0·2
2·0	14·0	10·80	0·6765	5·0185	0·2
2·1	15·6	11·73	0·7125	5·2362	0·2
2·2	17·4	12·69	0·7469	5·5129	0·1
2·3	19·4	13·81	0·7889	6·1126	0·2
2·4	21·5	14·85	0·8209	6·2846	0·2
2·5	23·8	15·96	0·8542	6·5276	0·3
2·6	26·3	17·26	0·8953	7·0784	0·3
2·7	29·0	18·37	0·9211	7·2568	0·4
2·8	31·9	19·68	0·9554	7·6692	0·4
2·9	35·0	20·94	0·9844	7·8883	0·5
3·0	38·4	22·27	1·0128	8·2616	0·5

Table 2. *Analytical constants for the absorption correction factor for cylindrical crystals*

μR	$A^*_{\theta=0}$	a	b	c	r.m.s. dev.
0·0	1·00	1·000	0·0000	0·0000	0·0%
0·1	1·18	1·180	0·0000	0·0000	0·0
0·2	1·40	1·503	0·0607	0·9750	0·4
0·3	1·65	1·615	0·0123	1·8912	0·5
0·4	1·95	1·979	0·0874	2·6509	0·1
0·5	2·29	2·320	0·1229	5·1682	0·1
0·6	2·69	2·721	0·1677	5·4849	0·1
0·7	3·16	3·177	0·2152	13·015	0·1
0·8	3·70	1·850	0·2731	0·2567	0·2
0·9	4·33	0·973	0·3312	0·3281	0·3
1·0	5·06	4·804	0·3538	2·6397	0·2
1·1	5·90	5·302	0·3823	2·1766	0·1
1·2	6·86	6·094	0·4393	2·7487	0·2
1·3	7·96	6·810	0·4792	3·0203	0·1
1·4	9·23	7·716	0·5327	3·5630	0·3
1·5	10·7	8·808	0·5971	4·3757	0·1
1·6	12·3	9·634	0·6276	4·3361	0·2
1·7	14·2	10·82	0·6845	4·9628	0·2
1·8	16·3	11·98	0·7310	5·3459	0·2
1·9	18·6	13·11	0·7701	5·5386	0·2
2·0	21·3	14·47	0·8184	6·0845	0·2
2·1	24·2	15·82	0·8600	6·4849	0·2
2·2	27·5	17·22	0·8997	6·8418	0·3
2·3	31·2	18·72	0·9405	7·3176	0·3
2·4	35·3	20·45	0·9887	7·8436	0·5

Our Tables 1 and 2 contain the following information in the consecutive columns: the value of μR for which the constants were computed; the value of $A^*_{\theta=0}$, a, b, c, and the r.m.s. value of $(A^*_{obs}-A^*_{calc})/A^*_{obs}$ over the 19 entries for the particular value of μR.

We are planning to extend this work to a five-constant formula (Moore, 1963) after a forthcoming change of computer.

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Estimation of error in the measured structure factor.

By S. C. ABRAHAMS, *Bell Telephone Laboratories, Incorporated, Murray Hill, New Jersey, U.S.A.*

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In a recent paper on automatic diffractometer programs (Cetlin & Abrahams, 1963), two formulae were given for computing the variance in the mean structure amplitude. In the notation of that paper, $\sigma^2(\bar{F}^2)$ gave the variance due to a Poisson distribution in the counting statistics and $V(\bar{F}^2)$ gave the variance due to those effects that are unequal with respect to reflections constrained by symmetry to be equivalent. It was also suggested that the variance ratio $V(\bar{F}^2)/\sigma^2(\bar{F}^2)$ be used as an indicator of systematic error. In practice, the F-distribution could not be interpreted satisfactorily. Table 1 (column 4) illustrates part of the very wide range found in a typical