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The Crystal and Molecular Structure of 1,3,4,6-Tetra-*O*-acetyl-2,5-*O*-methylene-D-mannitol: The Solid State Conformation of a 1,3-Dioxepane Ring

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$C_{15}H_{22}O_{10}$, monoclinic, $a = 10.000$, $b = 12.526$, $c = 8.193$ Å, $\gamma = 113.79^\circ$. Space group $P2_1$, 1338 independent reflexions, $R = 0.06$. The structure was solved with the tangent formula. The seven-membered ring is in the twist-chair conformation with the two O atoms in positions that relieve the main transannular interactions.

Introduction

There is little experimental information available about the conformations of unsubstituted seven-membered rings since pseudorotation is extremely facile. Strain-minimization calculations (Bocian, Picket, Rounds & Strauss, 1975) have predicted two pseudorotation families, the boat and chair, separated by an inversion barrier of ~ 34 kJ mol $^{-1}$. Each family has two extreme conformations; one is twisted (e.g. a twist-chair) with C_2 symmetry, the other is not twisted and has C_s

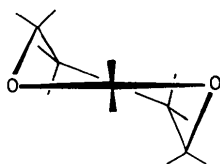
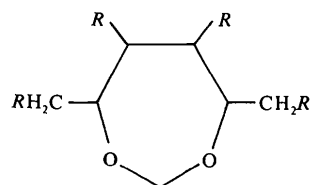


Fig. 1. Idealized C_3O_2 ring in the twist-chair conformation, showing C_2 symmetry.

symmetry. The calculations indicate that while the boat and twist-boat conformations have almost equal energy, the twist-chair is ~ 2 kJ mol $^{-1}$ more stable than the chair, and ~ 4 kJ mol $^{-1}$ more stable than the boat conformation.

The conformations of a number of substituted 1,3-dioxepane rings have been investigated in solution by 1H NMR (Grindley & Szarek, 1974) where it was concluded that the principal conformation is a twist-chair with the C_2 axis through the acetal C atom (Fig. 1). Presented here is the crystal structure of a closely related compound, 1,3,4,6-tetra-*O*-acetyl-2,5-*O*-methylene-D-mannitol (I).



(I) $R = CH_3COO$

Experimental

The crystals were prepared by the method of Ness, Hann & Hudson (1943) and had a m.p. of 117°C (literature m.p. 117–118°C).

Crystal data

$C_{15}H_{22}O_{10}$, $M_r = 363.3$, monoclinic, $a = 10.000 \pm 0.003$, $b = 12.526 \pm 0.002$, $c = 8.193 \pm 0.003$ Å, $\gamma = 113.79 \pm 0.01^\circ$, $D_m = 1.26$, $Z = 2$, $D_c = 1.281$ g cm $^{-3}$, Cu $K\alpha_1$ monochromatic radiation, $\lambda = 1.54051$ Å, $\mu = 8.43$ cm $^{-1}$. Systematic extinctions $00l$, $l = 2n + 1$. Space group $P2_1$. 1338 independent reflexions with $I > 3\sigma$ were measured on a Picker FACS-1 four-circle diffractometer.

Solution and refinement of structure

The phases of 147 reflexions with E values greater than 1.2 were determined by a multi-solution application of the tangent formula (Sheldrick, 1976). The E map calculated from the solution with the lowest Karle R factor had seven reasonably prominent maxima arranged in a seven-membered ring. The unique axis of the unit cell is perpendicular to the major plane through this ring and the false mirror symmetry often encountered in space group $P2_1$ in this case gives alternative positions for several of the atoms in the ring. A Fourier map phased on the most reasonable positions of the seven atoms revealed possible positions for the four side chains. These too occurred each with two alternative arrangements which were related by the false mirror. From these a trial structure was established that corresponded to the known structural formula, and as this was substantially correct the positions of all the heavy atoms were determined from the resultant difference Fourier synthesis. The final trial structure was refined by 'large' block least squares minimizing $\sum w(\Delta F)^2$; after three cycles with isotropic and two cycles with anisotropic temperature factors on all heavy atoms the conventional R was 0.09. The positions of all the H atoms were located from successive Fourier syntheses and when these were included with isotropic temperature factors the refinement converged at R 0.06. The weighting scheme used is given by: $W = [\sigma^2 |F_o|_{\text{abs}} + 0.726F_o^2]^{-1}$, where σ is the individual e.s.d. for each reflexion and was calculated from the diffractometer counting statistics. The final atomic coordinates are given in Table 1.* The atomic scattering factors used were those recorded in *International Tables for X-ray Crystallography* (1974) and were corrected for the real

* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32797 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

part of the anomalous dispersion effect. The interatomic distances and bond angles are given in Table 2. Fig. 2 shows the unique molecule and Fig. 3 illustrates

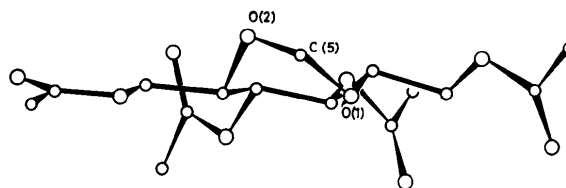


Fig. 2. The molecule viewed along a , the unit cell has been rotated by 3° about axes b and c .

Table 1. Atomic parameters ($\times 10^4$) with e.s.d.'s in parentheses

	x	y	z
C(1)	6744 (4)	8566 (3)	1793 (5)
C(2)	5280 (4)	7875 (3)	973 (5)
C(3)	4626 (4)	6563 (3)	1279 (0)
C(4)	5685 (4)	5978 (3)	1127 (5)
C(5)	7985 (5)	7289 (4)	2128 (7)
O(1)	7787 (3)	8161 (2)	1182 (4)
O(2)	6656 (3)	6375 (2)	2495 (4)
C(10)	7280 (5)	9836 (3)	1333 (6)
C(11)	9593 (5)	11364 (4)	1471 (7)
C(12)	10904 (6)	11932 (5)	2528 (12)
O(10)	8617 (3)	10451 (2)	2195 (4)
O(11)	9440 (4)	11714 (4)	177 (7)
C(20)	3772 (6)	8911 (4)	539 (7)
C(21)	2659 (6)	9262 (6)	1347 (9)
O(20)	4204 (3)	8275 (2)	1567 (4)
O(21)	4273 (6)	9196 (5)	-786 (6)
C(30)	2127 (5)	5390 (5)	649 (8)
C(31)	1062 (7)	4983 (6)	-727 (11)
O(30)	3468 (3)	6066 (2)	106 (4)
O(31)	1878 (5)	5108 (5)	2046 (7)
C(40)	4904 (4)	4658 (3)	1254 (6)
C(41)	5568 (4)	3068 (3)	1025 (6)
C(42)	6761 (6)	2693 (5)	693 (9)
O(40)	6009 (3)	4217 (2)	955 (4)
O(41)	4329 (5)	2429 (3)	1311 (9)
H(1)	6664	8391	2975
H(2)	5276	7979	-178
H(3)	4368	6505	2347
H(4)	6125	6477	183
H(5)	8446	7684	3176
H(6)	8590	6955	1468
H(10)	7434	9992	170
H(11)	6648	240	1646
H(40)	4021	4447	562
H(41)	4510	4454	2363
H(121)	1170	2741	2734
H(122)	1887	2290	2048
H(123)	796	1174	3052
H(211)	2054	8867	2317
H(212)	2760	9510	2512
H(213)	1660	8738	887
H(311)	1095	5876	-591
H(312)	1262	4737	-1777
H(313)	334	4274	-909
H(411)	6847	1842	455
H(412)	7699	3430	437
H(413)	7338	2723	1652

Table 2. *Interatomic distances (Å) and interbond angles (°)*

C(1)—O(1)	1.422 (6)	C(11)—O(11)	1.181 (8)
C(1)—C(2)	1.524 (5)	C(11)—C(12)	1.490 (9)
C(1)—C(10)	1.507 (6)	C(20)—O(20)	1.344 (7)
C(2)—C(3)	1.524 (5)	C(20)—O(21)	1.188 (7)
C(2)—O(20)	1.442 (6)	C(20)—C(21)	1.506 (10)
C(3)—C(4)	1.517 (6)	C(30)—O(30)	1.341 (5)
C(3)—O(30)	1.439 (4)	C(30)—O(31)	1.194 (9)
C(4)—C(40)	1.521 (5)	C(30)—C(31)	1.493 (10)
C(4)—O(2)	1.434 (5)	C(40)—O(40)	1.442 (6)
C(5)—O(1)	1.417 (6)	C(41)—O(40)	1.325 (5)
C(5)—O(2)	1.393 (4)	C(41)—O(41)	1.200 (6)
C(10)—O(10)	1.432 (5)	C(41)—C(42)	1.472 (9)
C(11)—O(10)	1.308 (5)		

the molecular packing. All calculations were computed with the Sheldrick (1976) system.

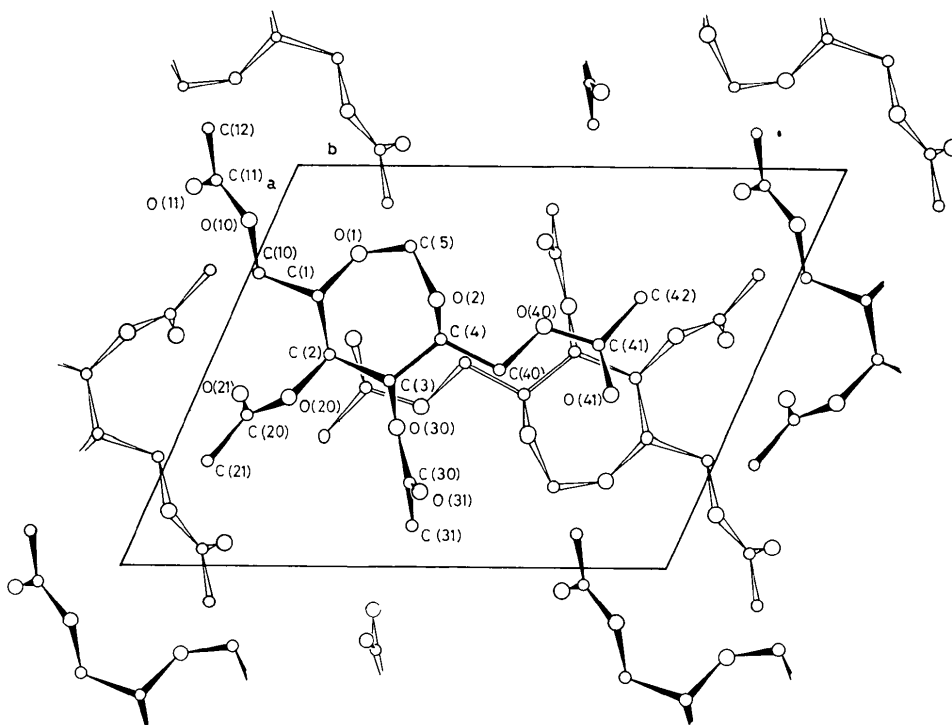
Results and discussion

The crystal contains isolated units of (I) with the mean plane of the ring nearly perpendicular to the 2_1 axis.

Table 3. *Torsional angles (°)*

Column 1 contains the angles for the present compound, column 2 refers to an ideal cycloheptane molecule in the twist-chair conformation (Flapper & Romers, 1975).

	(1)	(2)
C(2)—C(1)—O(1)	108.5 (3)	
C(2)—C(1)—C(10)	109.9 (4)	
O(1)—C(1)—C(10)	106.8 (3)	
C(1)—C(2)—C(3)	115.8 (3)	
C(1)—C(2)—O(20)	109.6 (3)	
C(3)—C(2)—O(20)	105.3 (3)	
C(2)—C(3)—C(4)	115.3 (3)	
C(2)—C(3)—O(30)	106.1 (3)	
C(4)—C(3)—O(30)	109.4 (3)	
C(3)—C(4)—O(2)	106.0 (3)	
C(3)—C(4)—C(40)	111.6 (3)	
O(2)—C(4)—C(40)	107.6 (3)	
O(1)—C(5)—O(2)	111.6 (4)	
C(1)—O(1)—C(5)	115.6 (3)	
C(4)—O(2)—C(5)	113.9 (3)	
C(1)—C(10)—O(10)	107.6 (4)	
C(10)—O(10)—C(11)	116.9 (4)	
O(10)—C(11)—O(11)	124.6 (4)	
O(10)—C(11)—C(12)	110.9 (5)	
O(11)—C(11)—C(12)	124.4 (5)	
C(2)—O(20)—C(20)	117.2 (4)	
O(20)—C(20)—O(21)	123.6 (6)	
O(20)—C(20)—C(21)	110.5 (5)	
O(21)—C(20)—C(21)	125.8 (6)	
C(3)—O(30)—C(30)	118.5 (4)	
O(30)—C(30)—C(31)	111.0 (5)	
O(30)—C(30)—O(31)	122.8 (5)	
O(31)—C(30)—C(31)	126.1 (5)	
C(4)—C(40)—O(40)	105.6 (3)	
C(40)—O(40)—C(41)	116.0 (3)	
O(40)—C(41)—O(41)	122.3 (5)	
O(40)—C(41)—C(42)	112.4 (4)	
O(41)—C(41)—C(42)	125.3 (5)	
C(1)—O(1)—C(5)—O(2)	50.2	37.2
C(2)—C(1)—O(1)—C(5)	-94.5	-84.0
C(3)—C(2)—C(1)—O(1)	61.5	66.8
C(4)—C(3)—C(2)—C(1)	-45.1	-47.4
O(2)—C(4)—C(3)—C(2)	69.9	66.8
C(5)—O(2)—C(4)—C(3)	-98.5	-84.0
O(1)—C(5)—O(2)—C(4)	45.6	37.2
C(40)—C(4)—C(3)—O(30)	-53.8	
O(30)—C(3)—C(2)—O(20)	72.4	
O(20)—C(2)—C(1)—C(10)	-63.2	
C(10)—O(10)—C(11)—O(11)	0.5	
C(1)—C(10)—O(10)—C(11)	148.1	
C(2)—O(20)—C(20)—O(21)	-3.4	
C(3)—O(30)—C(30)—O(31)	-6.1	
C(4)—C(40)—O(40)—C(41)	179.3	
C(40)—O(40)—C(41)—O(41)	0.3	

Fig. 3. The unit cell projected along *c*.

The four substituents on the ring are equatorial with the planes of three of the acetyl groups approximately perpendicular to the ring plane (Fig. 2). The plane of the fourth acetyl group is constrained to be nearly parallel with that of the ring, since this group passes over the molecule related by a screw axis (Fig. 3).

The conformation of the seven-membered ring is very close to a twist-chair (Table 3) and should therefore contain a C_2 axis. From Table 4 (planes 1, 2) it can be seen that there is almost a C_2 axis in the ring which passes through C(5) and bisects the C(2)–C(3) bond, so the prominent conformation of this type of molecule in solution (Grindley & Szarek, 1974) is maintained in the solid. One alternative description of the ring conformation has the five C atoms approximately coplanar, with one O well above and the other well below this plane (plane 3). In a C_7 ring of this conformation it would be the axial substituents of the two out-of-plane atoms which would give the closest transannular contacts and in the present compound it is no surprise, therefore, to find that these out-of-plane atoms are O atoms which have no substituents.

The structures of one monocyclic substituted cycloheptane and some monocyclic oxacycloheptanes have been determined (Flapper & Romers, 1975; Beale, Stephenson & Stevens, 1971) and their conformations are intermediate between the chair and twist-chair form. The X-ray structure of cycloheptane is not known, but the structure of an azacycloheptane ($C_6H_{14}N^+Cl^-$) has recently been determined (Cameron & Scheeren, 1977). The projection of this molecule on the least-squares plane through all the seven atoms is also given in Table 4. It can be seen that the twofold axis is not so prominent, which suggests that the relief of the transannular interaction significantly affects the conformation that these molecules adopt. Since none of the conformations of seven-membered rings in monocyclic compounds with known structures are in the boat

family, it seems unlikely that the recent suggestion (Bocian *et al.*, 1975) that the boat and chair families have equal populations at 300 K is correct.

The large difference in the internal ring interbond angles at C(2) and C(3), 115.8 and 115.3°, compared with those at C(1) and C(4), 108.5 and 106.0°, is probably caused by σ -bond repulsions (Cameron & Prout, 1969), where, for example, the oxygen atom O(20) polarizes the O(20)–C(2) bond, pulls the electrons towards itself and thus reduces the repulsion between the σ electrons of that bond and those of the C(2)–C(1) and C(2)–C(3) bonds. Thus the C(1)–C(2)–C(3) bond angle will be the largest of the three formed by the 'heavy' atoms at C(2). Similarly, the bond angles C(3)–C(4)–C(40) and C(2)–C(1)–C(10) are also the largest of the three formed at C(4) and C(1) as a result of the polarization of the O(2)–C(4) and O(1)–C(1) bonds respectively. Consequently, the internal ring angles at C(1) and C(4) will be less than 109.5° and smaller than those at C(2) and C(3).

The internal ring angles, mean 112.4°, are smaller than those observed in dimeric cycloheptane peroxide, mean 115.3° (Groth, 1967), and in azacycloheptane, mean 116.0° (Cameron & Scheeren, 1977).

The dimensions of the molecule are as expected with the exception of the bond lengths at the ring O atoms of which two are significantly different, O(2)–C(5) 1.393 (4) and O(2)–C(4) 1.434 (5) Å. The short transannular O–H contacts are O(1)···H(4) 2.25, O(2)···H(3) 2.36 Å. The effect of the O(1)···H(4) interaction is to require a bond lengthening somewhere along the chain C(4)–O(2)–C(5)–O(1) and for the O(2)···H(3) interaction, a lengthening along the chain O(2)–C(4)–C(3). The only bond common to both is C(4)–O(2) which is the longest of the four C–O ring bonds, while the bonds on either side, C(4)–C(3) and O(2)–C(5), are respectively the shortest of the C–C and C–O bonds. An alternative explanation for short bonds between acetal C atoms and their O atoms, in terms of bond strengthening by back bonding from oxygen lone pairs into an orbital of the inductively electron-depleted C, has been given (Jeffery, Pople & Radom, 1972).

Table 4. *Atomic planes*

Perpendicular distance from least-squares planes through the atoms is marked with an asterisk. Plane 2 passes through atom C(5), bisects the C(2)–C(3) bond and is perpendicular to plane 1. Plane 4 is for azacyclo ($C_6H_{14}N^+Cl^-$).

Plane	1	2	3	4	
C(1)	0.47	–1.46	0.10*	0.35*	C(1)'
C(2)	0.00*	–0.76(*)	–0.22*	–0.05*	N(1)'
C(3)	0.00*	0.76(*)	0.22*	0.09*	C(3)'
C(4)	–0.58	1.38	–0.10*	–0.42*	C(4)'
O(2)	0.35	1.10	0.77	0.48*	C(5)'
C(5)	0.00*	0.00*	0.16	0.03*	C(6)'
O(1)	–0.42	–1.10	–0.58	–0.48*	C(7)'
C(10)	0.37	–0.295	–0.42	0.11	
O(20)	0.87	–1.11	0.46	0.78	
O(30)	–0.76	1.19	–0.45	–0.63	
C(40)	–0.69	2.89	0.21	–0.39	

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Structure Cristalline du Fluoroindate de Potassium KIn_2F_7

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(Reçu le 4 mai 1977, accepté le 24 mai 1977)

KIn_2F_7 is monoclinic, with parameters $a = 10.753$, $b = 8.131$, $c = 6.609$ Å, $\beta = 90.71^\circ$, space group $P2_1/m$. The structure was solved by three-dimensional Patterson and Fourier techniques and refined by least-squares procedures to a conventional $R = 0.047$ for 708 independent reflexions. The idealized structure arises when parallel chains of edge-sharing regular pentagonal bipyramids are fused together by corner-sharing in the two directions perpendicular to the chains. A three-dimensional network is then produced in the tunnels of which K atoms are located. Structural relations with ReO_3 and $\alpha\text{-U}_3\text{O}_8$ structures are discussed.

Le fluorure d'indium InF_3 forme avec la plupart des fluorures d'éléments monovalents une série de fluoroindates de formule générale $M_x\text{InF}_{3+x}$ (Grannec, Champarnaud-Mesjard & Portier, 1970; Grannec, Champarnaud-Mesjard, Costy, Cousseins & Gaudreau, 1972; Champarnaud-Mesjard, Grannec & Gaudreau, 1974). Aucune de ces phases n'a jusqu'ici fait l'objet d'une étude structurale approfondie. Or l'examen attentif des spectres X de poudre et des paramètres cristallins des composés correspondant aux termes $x = 0,33$ ($M\text{In}_3\text{F}_{10}$), $x = 0,50$ ($M\text{In}_2\text{F}_7$), $x = 0,66$ ($M_2\text{In}_3\text{F}_{11}$) permet raisonnablement d'envisager, d'une part l'isotypie des phases relatives à une même composition, d'autre part l'existence de liens structuraux étroits entre phases de compositions différentes. Nous avons donc entrepris une étude cristallographique complète de l'ensemble de ces phases.

Les premiers résultats, relatifs aux phases $M\text{In}_3\text{F}_{10}$, ont fait l'objet d'une publication récente (Champarnaud-Mesjard, Mercurio & Frit, 1977); dans le présent article sont reportés ceux relatifs aux phases $M\text{In}_2\text{F}_7$ et plus précisément au fluoroindate de potassium KIn_2F_7 .

Obtention d'un monocristal – constantes cristallographiques de KIn_2F_7

Parmi les composés $M\text{In}_2\text{F}_7$ isolés ($M = \text{K}, \text{Rb}, \text{NH}_4$) seul KIn_2F_7 était susceptible de donner des monocristaux bien formés, les deux autres phases se décomposant avant fusion.

Après plusieurs essais, des cristaux prismatiques de la phase KIn_2F_7 ont été obtenus par fusion à 840°C , suivie d'un refroidissement lent, en tube de platine scellé, d'un mélange $\text{KF}-2\text{InF}_3$. L'un d'eux de dimensions convenables ($0,18 \times 0,18 \times 0,30$ mm) a été sélectionné en vue d'une étude cristallographique complète. Cette dernière, effectuée à l'aide des techniques de Laue, Bragg, Buerger et Weissenberg, a montré que KIn_2F_7 cristallisait dans le système monoclinique (pseudo-orthorhombique). Les constantes cristallographiques de KIn_2F_7 sont portées au Tableau 1.

La règle d'existence relevée pour l'ensemble des taches hkl de diffraction ($0k0$, $k = 2n$), est compatible avec les seuls groupes $P2_1$ et $P2_1/m$. Cependant, comme dans le cas de $\text{RbIn}_3\text{F}_{10}$, elle pourrait fort bien n'être qu'une conséquence de la quasi extinction générale constatée sur les strates $\{(010)\}_n$ d'ordre n impair (extinction parfaitement justifiée comme nous le verrons plus loin, par la répartition des atomes dans la maille cristalline); aussi nous n'avons pas exclu *a priori* les groupes $P2$ et $P2/m$. Par ailleurs, l'existence pour l'ensemble des taches de diffraction hkl d'une pseudo-extinction (hkl , $h + k + l \neq 2n$) permet de penser que les atomes métalliques sont très vraisemblablement situés aux noeuds d'un réseau pseudo-orthorhombique de mode I.

Détermination de la structure

En raison de la trop faible intensité générale des taches de diffraction relatives aux strates $\{(010)\}_n$ d'ordre n