The Crystal Structure of D-Mannitol Tris(benzeneboronic) Ester, $C_{24}H_{23}B_3O_6$

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D-Mannitol tris(benzeneboronic) ester, $C_{24}H_{23}B_3O_6$, is orthorhombic, space group $P2_12_12_1$, with $a = 13\cdot991$ (6), $b = 26\cdot842$ (4), $c = 6\cdot095$ (3) Å, $Z = 4$. The structure was solved by direct methods and refined by full-matrix least squares to $R_w = 0\cdot040$ ($0\cdot032$ omitting 'unobserveds'). The analysis establishes the compound as mannitol tris(1,2:3,4:5,6-benzeneboronic) ester with 1,2,3-dioxaborolane rings resulting from the reaction of boronic acid with 1,2-dihydroxy groups.

Introduction

D-Mannitol tris(benzeneboronic) ester was prepared from D-mannitol and benzeneboronic acid in aqueous methanol (Kuivilla, Keough & Soboczenski, 1954). Though the accurate structure of the compound could not be determined, the presence of five, six or seven-membered boronic esters was assumed (Sugihara & Bowman, 1958).

After attempts to establish the structure by chemical methods had failed, because of the easy transesterification of the boron ester and the strong tendency to form the final product (Zabrocki, 1971), the substance was examined by ^{13}C NMR spectroscopy; this also yielded results which could not be interpreted unambiguously. Besides these configurative questions, the bonding conditions of B were of interest in this compound since the substance, contrary to the normal highly hydrolysis-sensitive boron esters, can be synthesized in aqueous solution. In order to solve these problems an X-ray structure analysis has been undertaken.

Experimental

D-Mannitol tris(benzeneboronic) ester crystallizes as clear colourless needles. The crystal selected for X-ray analysis was cut to $0\cdot2 \times 0\cdot2 \times 0\cdot2$ mm. Weissenberg photographs established the space group as $P2_12_12_1$ from the systematic absences $h00$ with h odd, $0k0$ with k odd and $00l$ with l odd. The diffraction data were collected on an automatic four-circle diffractometer (Syntex $P2_1$) with Mo $K\alpha$ radiation ($\lambda = 0\cdot71069$ Å)

and a graphite monochromator ($2\theta = 12\cdot2°$). Unit-cell parameters were determined by least squares from the adjusted angular settings of 25 reflexions: $a = 13\cdot991$ (6), $b = 26\cdot842$ (4), $c = 6\cdot095$ (3) Å; $V = 2289\cdot0$ ($1\cdot8$) Å^3.

The asymmetric unit consists of one molecule of $C_{24}H_{23}B_3O_6$. With a molecular weight of $437\cdot0$, $D_x = 1\cdot25$ g cm^{-3}. The intensity measurements were carried out in the $\theta–2\theta$ mode with a $1\cdot4°$ plus (α_1, α_2)-dispersion scan range. The total background counting time equalled the time spent for the peak count. Up to a maximum value of $2\theta = 50°$, 4492 reflexions were recorded, resulting in a set of 2145 unique reflexions, 955 of which were regarded as unobserved ($I < 3\sigma$). The internal agreement index of the data set based on the deviations of the $|F_h|$ of equivalent reflexions from their means, $|\bar{F}_h|$, was

$$Rf = \sum_h \sum_i ||\bar{F}_h| - |F_{h,i}||/\sum_h \sum_i |F_{h,i}| = 0\cdot08.$$

No absorption corrections were applied ($\mu = 0\cdot902$ cm^{-1}).

Structure determination

The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971) ($300|E| \geq 1\cdot38$, 2000 Σ_2 relationships, $\chi_{hh'} \geq 6\cdot53$). For the set of phases with the highest CFOM ($2\cdot92$), an E map was calculated. From the peak-search procedure, the 50 highest peaks were retained, of which 33 could be identified as the C, O and B atoms. At this stage the overall R based on full-matrix least-squares refinement of the scale factor, overall temperature factor and atomic positional

parameters was 0·22. Another least-squares cycle with individual isotropic temperature factors reduced R to 0·18. With anisotropic temperature factors R dropped to 0·13. The reflexions were weighted with an adjustable Cruickshank scheme. The final weights were: $w = 1·0$ for $|F_o| > 25·0$; and $w = 0·04|F_o|$ for $|F_o| \leq 25·0$.

The positions of the 23 H atoms were calculated from stereochemical considerations and assigned the isotropic temperature factors of the carrier atoms. Only the positional parameters of the H atoms were refined. An isotropic extinction factor (Zachariasen, 1963) was refined, the final value being $g = 1·4 \times 10^{-6}$. Since there were 366 parameters, refinement had to be carried out in overlapping cycles. Refinement was stopped when the shifts were below the standard deviations. The final R(overall) = 0·102 (0·048 omitting 'unobserveds') and $R_w = 0·040$ (0·032 omitting 'unobserveds').*

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* A list of structure factors is available from the authors and has also been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32079 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Discussion

This analysis establishes the compound as mannitol tris(1,2 : 3,4 : 5,6-benzeneboronic) ester. Thus no six-membered 1,3-dihydroxyboronate esters were formed, but all three boronic acid molecules reacted with 1,2-dihydroxy groups to yield five-membered 1,3,2-dioxaborolane rings.

An $ORTEP$ drawing of the molecule is shown in Fig. 1 (Johnson, 1965). The atomic parameters and temperature factors are listed in Tables 1 and 2. The interatomic distances and angles at the heavy atoms are given in Table 3 and illustrated schematically with the numbering scheme of the atoms in Fig. 2(a) and (b). The 23 C—H distances vary from 0·95 to 1·19 Å [mean 1·06 (6) Å]. The C—C—C angles in the mannitol group vary from 111·7 to 113·3° [mean 112·8 (5)°]. The C—C distances of this group range from 1·517 to 1·557 Å [mean 1·532 (9) Å]. The C—C—C angles in the three phenyl rings are from 118·3 to 122·7° [mean 120·0 (6)°]. The C—C distances in these rings lie in the expected range of 1·365 to 1·418 Å [mean 1·390 (10) Å].

Table 1. *Positional and thermal parameters* ($\times 10^4$ *for heavy atoms*), *with standard deviations in parentheses*

The expression for the temperature factor is: $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
C(1)	738 (6)	2467 (2)	11132 (14)	101 (7)	20 (1)	416 (32)	6 (3)	87 (13)	−3 (6)
C(2)	1080 (5)	2273 (2)	8896 (11)	57 (5)	14 (1)	333 (24)	−0 (2)	20 (10)	6 (5)
C(3)	2016 (4)	1981 (2)	9023 (11)	51 (4)	10 (1)	321 (24)	−1 (2)	13 (9)	7 (4)
C(4)	2340 (4)	1792 (2)	6724 (10)	57 (4)	10 (1)	345 (23)	−5 (2)	2 (8)	12 (4)
C(5)	3400 (4)	1865 (2)	6308 (11)	59 (5)	12 (1)	321 (25)	−5 (2)	13 (9)	13 (4)
C(6)	3709 (5)	1693 (2)	4034 (12)	79 (6)	12 (1)	367 (27)	−3 (2)	49 (12)	2 (4)
C(7)	1265 (4)	3661 (2)	8032 (10)	58 (4)	15 (1)	291 (21)	4 (2)	−0 (10)	0 (4)
C(8)	1103 (5)	4064 (3)	9439 (12)	82 (6)	19 (1)	444 (30)	3 (2)	−4 (12)	−9 (6)
C(9)	1341 (5)	4550 (2)	8735 (12)	105 (6)	16 (1)	557 (33)	3 (2)	26 (14)	−8 (5)
C(10)	1741 (5)	4629 (3)	6724 (15)	77 (6)	16 (1)	690 (43)	4 (2)	34 (14)	6 (7)
C(11)	1909 (6)	4240 (3)	5298 (15)	96 (6)	20 (1)	465 (33)	4 (2)	33 (13)	20 (6)
C(12)	1679 (5)	3754 (2)	5997 (11)	59 (5)	18 (1)	397 (29)	−1 (2)	11 (10)	3 (5)
C(13)	3833 (4)	3095 (2)	3389 (10)	54 (4)	15 (1)	271 (20)	−4 (2)	−8 (9)	1 (4)
C(14)	4254 (5)	3433 (2)	4815 (11)	65 (5)	15 (1)	329 (25)	0 (2)	−1 (10)	2 (5)
C(15)	4454 (5)	3925 (2)	4099 (14)	85 (6)	17 (1)	407 (30)	−3 (2)	−2 (11)	−16 (5)
C(16)	4196 (4)	4059 (2)	2021 (11)	54 (4)	16 (1)	511 (29)	−4 (2)	19 (10)	12 (5)
C(17)	3753 (5)	3738 (2)	598 (11)	88 (5)	14 (1)	314 (23)	2 (2)	−2 (11)	14 (4)
C(18)	3579 (4)	3245 (2)	1302 (11)	60 (4)	16 (1)	334 (24)	−6 (2)	29 (9)	−12 (4)
C(19)	1567 (3)	603 (2)	9561 (10)	41 (4)	12 (1)	376 (22)	−1 (1)	−6 (8)	5 (4)
C(20)	1599 (5)	214 (2)	8033 (12)	71 (5)	14 (1)	337 (25)	−0 (2)	5 (11)	11 (5)
C(21)	1241 (5)	−252 (2)	8570 (13)	69 (5)	14 (1)	423 (31)	−5 (2)	4 (12)	−4 (5)
C(22)	848 (6)	−332 (3)	10605 (16)	100 (6)	12 (1)	532 (36)	−3 (2)	40 (13)	19 (6)
C(23)	840 (6)	36 (3)	12169 (15)	96 (7)	16 (1)	451 (34)	0 (2)	29 (12)	29 (6)
C(24)	1193 (5)	513 (2)	11644 (12)	66 (5)	14 (1)	362 (27)	0 (2)	31 (11)	−1 (4)
B(1)	1103 (6)	3121 (3)	8829 (14)	45 (5)	19 (1)	349 (32)	1 (2)	23 (12)	21 (6)
B(2)	3704 (5)	2542 (3)	4160 (13)	37 (5)	15 (1)	297 (27)	−9 (2)	−8 (10)	0 (5)
B(3)	1875 (5)	1145 (3)	8850 (14)	53 (6)	15 (1)	311 (30)	6 (2)	−7 (11)	8 (6)
O(1)	812 (3)	3012 (2)	10910 (8)	106 (4)	14 (1)	410 (20)	−1 (1)	36 (8)	−4 (3)
O(2)	1228 (3)	2706 (1)	7520 (7)	84 (3)	13 (1)	361 (17)	9 (1)	24 (7)	6 (3)
O(3)	3592 (3)	2399 (1)	6285 (7)	66 (3)	15 (1)	266 (15)	−11 (1)	6 (6)	9 (3)
O(4)	3724 (3)	2147 (1)	2707 (7)	86 (4)	13 (1)	323 (16)	−6 (1)	15 (7)	−2 (3)
O(5)	1830 (3)	1537 (1)	10278 (7)	75 (3)	12 (1)	309 (15)	−2 (1)	14 (6)	5 (3)
O(6)	2167 (3)	1261 (1)	6804 (7)	70 (3)	11 (1)	327 (15)	−7 (1)	20 (6)	−5 (3)

Table 2. *The positional parameters of the hydrogen atoms* ($\times 10^3$) *and isotropic thermal parameters, with standard deviations in parentheses*

	x	y	z	B (Å²)
H1(C1)	115 (5)	238 (2)	1255 (11)	5.33
H2(C1)	6 (4)	241 (2)	1150 (11)	3.30
H(C2)	52 (4)	202 (2)	790 (10)	4.43
H(C3)	261 (3)	220 (2)	966 (10)	3.52
H(C4)	197 (3)	198 (2)	529 (8)	2.27
H(C5)	388 (4)	173 (2)	774 (10)	4.26
H1(C6)	324 (4)	146 (2)	339 (10)	2.80
H2(C6)	449 (4)	152 (2)	393 (11)	4.21
H(C8)	74 (5)	404 (3)	1100 (12)	6.23
H(C9)	112 (4)	484 (2)	990 (9)	3.10
H(C10)	198 (4)	500 (2)	610 (13)	6.55
H(C11)	202 (5)	425 (3)	371 (12)	5.40
H(C12)	159 (4)	350 (2)	493 (8)	2.76
H(C14)	434 (4)	332 (2)	645 (11)	4.72
H(C15)	476 (4)	413 (2)	540 (11)	5.23
H(C16)	447 (3)	441 (2)	137 (9)	3.32
H(C17)	348 (4)	385 (2)	−111 (10)	4.87
H(C18)	341 (4)	300 (2)	27 (9)	3.76
H(C20)	167 (5)	32 (3)	645 (12)	5.43
H(C21)	118 (5)	−50 (2)	728 (11)	4.48
H(C22)	70 (5)	−67 (2)	1115 (12)	5.32
H(C23)	52 (4)	−3 (2)	1393 (12)	4.28
H(C24)	111 (4)	77 (2)	1280 (11)	4.60

The results of least-squares planes calculations are given in Table 4. The phenyl rings (planes G, H and I) are planar with a mean deviation of 0·008 Å for the C
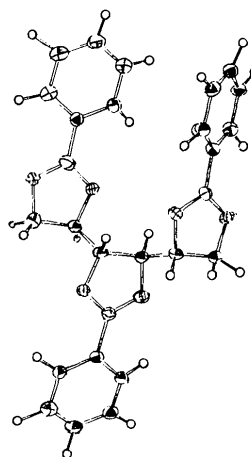

Fig. 1. *ORTEP* drawing of the mannitol tris(benzeneboronic) ester molecule.

Table 3. *Bond distances* (Å) *and angles* (°)

Standard deviations in parentheses are for the last significant digit.

C(1)—C(2)	1.534 (11)	B(1)—O(1)	1.363 (0)	C(2)—C(1)—O(1)	103.5 (6)	C(15)—C(16)—C(17)	122.7 (6)
C(1)—O(1)	1.471 (8)	B(1)—O(2)	1.383 (0)	C(1)—C(2)—C(3)	113.3 (6)	C(16)—C(17)—C(18)	118.5 (6)
C(2)—C(3)	1.528 (9)	B(2)—O(3)	1.360 (0)	C(1)—C(2)—O(2)	106.7 (5)	C(13)—C(18)—C(17)	120.5 (6)
C(2)—O(2)	1.446 (6)	B(2)—O(4)	1.384 (0)	C(3)—C(2)—O(2)	108.5 (5)	C(20)—C(19)—C(24)	119.1 (5)
C(3)—C(4)	1.557 (9)	B(3)—O(5)	1.364 (0)	C(2)—C(3)—C(4)	111.7 (5)	C(20)—C(19)—B(3)	120.0 (5)
C(3)—O(5)	1.440 (6)	B(3)—O(6)	1.348 (0)	C(2)—C(3)—O(5)	107.4 (5)	C(24)—C(19)—B(3)	120.8 (4)
C(4)—C(5)	1.517 (8)	C(1)—H1(C1)	1.06 (7)	C(4)—C(3)—O(5)	105.1 (4)	C(19)—C(20)—C(21)	120.6 (7)
C(4)—O(6)	1.448 (5)	C(1)—H2(C1)	0.99 (6)	C(3)—C(4)—C(5)	113.2 (5)	C(20)—C(21)—C(22)	119.8 (7)
C(5)—C(6)	1.524 (10)	C(2)—H(C2)	1.19 (6)	C(3)—C(4)—O(6)	103.9 (4)	C(21)—C(22)—C(23)	121.2 (7)
C(5)—O(3)	1.456 (6)	C(3)—H(C3)	1.08 (5)	C(5)—C(4)—O(6)	107.2 (4)	C(22)—C(23)—C(24)	119.5 (8)
C(6)—O(4)	1.460 (6)	C(4)—H(C4)	1.15 (5)	C(4)—C(5)—C(6)	113.0 (5)	C(19)—C(24)—C(23)	119.9 (6)
C(7)—C(8)	1.400 (9)	C(5)—H(C5)	1.16 (6)	C(4)—C(5)—O(3)	108.0 (4)	O(1)—B(1)—C(7)	122.5 (2)
C(7)—C(12)	1.391 (9)	C(6)—H1(C6)	1.00 (5)	C(6)—C(5)—O(3)	103.6 (5)	O(1)—B(1)—O(2)	113.6 (0)
C(7)—B(1)	1.546 (5)	C(6)—H2(C6)	1.17 (6)	C(5)—C(6)—O(4)	104.8 (4)	O(2)—B(1)—C(7)	123.9 (2)
C(8)—C(9)	1.414 (9)	C(8)—H(C8)	1.07 (7)	C(8)—C(7)—C(12)	118.3 (5)	O(3)—B(2)—C(13)	124.7 (2)
C(9)—C(10)	1.367 (11)	C(9)—H(C9)	1.09 (5)	C(8)—C(7)—B(1)	120.6 (5)	O(3)—B(2)—O(4)	113.1 (0)
C(10)—C(11)	1.375 (12)	C(10)—H(C10)	1.10 (7)	C(12)—C(7)—B(1)	120.7 (5)	O(4)—B(2)—C(13)	122.2 (2)
C(11)—C(12)	1.408 (10)	C(11)—H(C11)	0.97 (7)	C(7)—C(8)—C(9)	119.2 (6)	O(5)—B(3)—C(19)	123.2 (2)
C(13)—C(14)	1.389 (9)	C(12)—H(C12)	0.96 (5)	C(8)—C(9)—C(10)	120.8 (6)	O(5)—B(3)—O(6)	115.2 (0)
C(13)—C(18)	1.382 (9)	C(14)—H(C14)	1.06 (7)	C(9)—C(10)—C(11)	121.3 (7)	O(6)—B(3)—C(19)	121.5 (2)
C(13)—B(2)	1.566 (5)	C(15)—H(C15)	1.05 (7)	C(10)—C(11)—C(12)	118.2 (8)	B(1)—O(1)—C(1)	108.6 (3)
C(14)—C(15)	1.418 (9)	C(16)—H(C16)	1.09 (5)	C(7)—C(12)—C(11)	122.1 (6)	B(1)—O(2)—C(2)	107.1 (3)
C(15)—C(16)	1.367 (11)	C(17)—H(C17)	1.13 (6)	C(14)—C(13)—C(18)	119.6 (5)	B(2)—O(3)—C(5)	108.1 (3)
C(16)—C(17)	1.367 (9)	C(18)—H(C18)	0.95 (5)	C(14)—C(13)—B(2)	118.7 (5)	B(2)—O(4)—C(6)	106.6 (3)
C(17)—C(18)	1.412 (8)	C(20)—H(C20)	0.99 (7)	C(18)—C(13)—B(2)	121.6 (4)	B(3)—O(5)—C(3)	106.9 (2)
C(19)—C(20)	1.400 (9)	C(21)—H(C21)	1.04 (6)	C(13)—C(14)—C(15)	120.0 (6)	B(3)—O(6)—C(4)	108.0 (2)
C(19)—C(24)	1.391 (9)	C(22)—H(C22)	0.99 (6)	C(14)—C(15)—C(16)	118.6 (6)		
C(19)—B(3)	1.579 (5)	C(23)—H(C23)	1.17 (7)				
C(20)—C(21)	1.383 (9)	C(24)—H(C24)	1.01 (6)				
C(21)—C(22)	1.376 (12)						
C(22)—C(23)	1.373 (12)						
C(23)—C(24)	1.412 (10)						

atoms. The five-membered rings (planes A, B and C), consisting of one B, two O and two C atoms each, are fairly planar with a mean deviation of the atoms of 0·045 Å. The arrangements of the C and O around the B atoms (planes D, E and F) are essentially planar with

a mean deviation of the atoms of 0·004 Å. Hence it can be concluded that the formation of the substance in aqueous solution is not due to a tetravalent character of the B atoms, but to the low solubility of the compound in water (Sugihara & Bowman, 1958).

The planes A, B and C (five-membered rings) are approximately parallel, their distances apart being 1·5 Å $(A-C)$ and 1·3 Å $(B-C)$.

According to Jeffrey & Kim (1970), mannitol itself is in an extended, planar, zigzag chain configuration. In the title compound such a configuration of the mannitol chain is not possible since C(3) and C(4) form part of the five-membered ring system (plane C). Two sets of
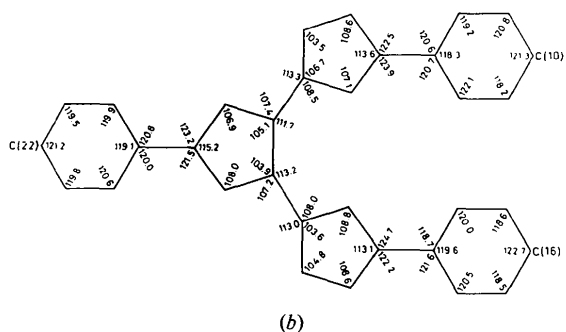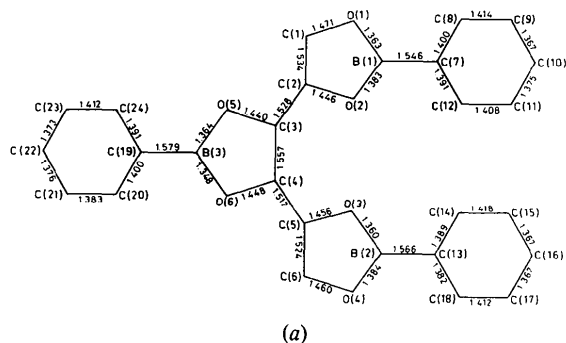

(a)

(b)

Fig. 2. (a) Numbering scheme and bond distances (Å). (b) Bond angles (°).
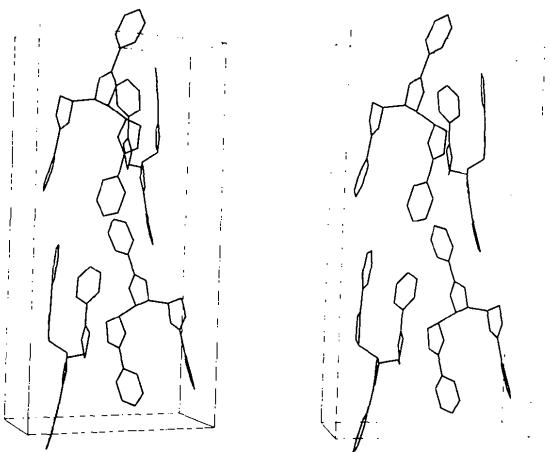

Fig. 3. *ORTEP* drawing of the arrangement of the molecules in the unit cell, approximately along [001].

Table 4. *Least-squares planes* (*deviations in* Å)

Plane A (five-membered ring)

C(1)	C(2)	B(1)	O(1)	O(2)
−0·026	0·036	0·018	0·007	−0·034

Plane B (five-membered ring)

C(5)	C(6)	B(2)	O(3)	O(4)
−0·112	0·109	−0·006	0·077	−0·068

Plane C (five-membered ring)

C(3)	C(4)	B(3)	O(5)	O(6)
−0·053	0·042	−0·021	0·048	−0·016

Plane D (atoms around boron)

C(7)	B(1)	O(1)	O(2)
−0·002	0·005	−0·002	−0·002

Plane E (atoms around boron)

C(13)	B(2)	O(3)	O(4)
0·004	−0·012	0·004	0·004

Plane F (atoms around boron)

C(19)	B(3)	O(5)	O(6)
−0·004	0·012	−0·004	−0·004

Plane G (phenyl ring)

C(7)	C(8)	C(9)	C(10)	C(11)	C(12)
−0·006	0·002	−0·002	0·006	−0·009	0·009

Plane H (phenyl ring)

C(13)	C(14)	C(15)	C(16)	C(17)	C(18)
0·009	−0·013	0·006	0·005	0·010	0·003

Plane I (phenyl ring)

C(19)	C(20)	C(21)	C(22)	C(23)	C(24)
−0·012	0·005	0·010	−0·017	−0·010	0·005

Plane J (part of mannitol chain)

C(1)	C(2)	C(3)	C(4)
0·002	−0·002	−0·002	0·002

Plane K (part of mannitol chain)

C(3)	C(4)	C(5)	C(6)
0·010	−0·010	−0·010	0·010

four atoms, C(1), C(2), C(3), C(4) and C(3), C(4), C(5), C(6), form planar zigzag chains (planes J and K). These chains are twisted against each other by 43° around C(3)–C(4).

The planes G and I (phenyl rings) are almost parallel to each other with an angular deviation of 10°; and although the planes G and H can be regarded as equivalent, the latter is twisted along the boronic acid–phenyl ring axis. The angles included here are 39° (H–G) and 44° (H–I). This configuration affects the symmetry of the molecule significantly. If one assumes a similar configuration for the molecule in solution, then at least at elevated temperatures a degenerative transition caused by rotation of the phenyl rings G and I should be possible. Without this knowledge, a structure analysis of the compound by ^{13}C NMR spectroscopy based on the equivalence of C(1), C(2) and C(5), C(6) in the mannitol chain and the C atoms of the phenyl rings of planes G and H could have led to wrong conclusions. The results of ^{13}C NMR spectroscopic analysis will be reported elsewhere (Wulff, Zabrocki, Gupta, Kirfel & Will, 1977).

A stereoscopic view of the arrangement of the molecules in the unit cell, approximately along [001], is shown in Fig. 3.

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The Crystal Structure of the Triterpene Oxide Campanulin. A Comparative Study on a Strained Hydrocarbon Ring System

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The structure of campanulin, $C_{30}H_{50}O$, was solved by a tangent-refinement procedure and refined by full-matrix least squares. The final R based on 2290 F_o corrected for absorption was 0·039; R_w was 0·046. Campanulin is a friedelan-type triterpene with *cis*-fused rings D and E in the chair form. The conformation of this part of the molecule is highly strained, as borne out by a number of long C–C bonds, large valency angles and small torsion angles. The electronic structure of rings A, B and C is in close agreement with that of baccharis oxide [Mo, *Acta Cryst.* (1973), B29, 1796–1807]. R.m.s. and maximum differences over 21 pairs of C–C and C–O bonds in the two structures are only 0·004 and 0·010 Å; corresponding figures for 37 pairs of valency angles are 0·69 and 1·6° respectively. The results indicate that the e.s.d.'s from the least-squares refinement are realistic estimates. Since packing forces appear to be of minor significance for the molecular conformation, it is also suggested that the parameters obtained in these studies are good approximations to those of the isolated molecules.

Introduction

A triterpene oxide isolated from various *Rhododendron* species (Rangaswami & Sambamurthy,

1961*a*; Arthur & Hui, 1961) and *Dendropanax trifidus* Makino (Kimura, Hashimoto & Agata, 1960) has been varyingly named campanulin, epoxyglutinane and dendropanoxide. Rangaswami & Sambamurthy (1961*b*) showed that campanulin and epoxyglutinane are identical compounds. From chemical and spectro-

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