Table 1. *Final coordinates and equivalent isotropic thermal parameters of the non-hydrogen atoms, with their e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}(Å^2)
O(1)	0·7164 (2)	0·3773 (2)	0·2739 (1)	0·0541 (5)
O(2)	1·2833 (3)	0·3373 (2)	0·2305 (1)	0·0500 (5)
C(1)	0·8405 (3)	0·4503 (2)	0·2346 (1)	0·0409 (6)
C(2)	1·0305 (3)	0·5227 (3)	0·2706 (1)	0·0441 (6)
C(3)	1·2266 (3)	0·4915 (2)	0·2201 (1)	0·0459 (6)
C(4)	1·1918 (3)	0·5257 (3)	0·1332 (1)	0·0476 (7)
C(5)	1·0068 (3)	0·4374 (3)	0·0994 (1)	0·0440 (6)
C(6)	0·8092 (3)	0·4751 (3)	0·1469 (1)	0·0491 (7)
C(7)	1·0584 (4)	0·4868 (4)	0·3572 (2)	0·0633 (9)
C(8)	0·9704 (3)	0·4613 (3)	0·0118 (1)	0·0521 (7)
C(9)	0·9531 (5)	0·3431 (4)	−0·0370 (2)	0·067 (1)
C(10)	0·9535 (6)	0·6159 (4)	−0·0173 (2)	0·078 (1)

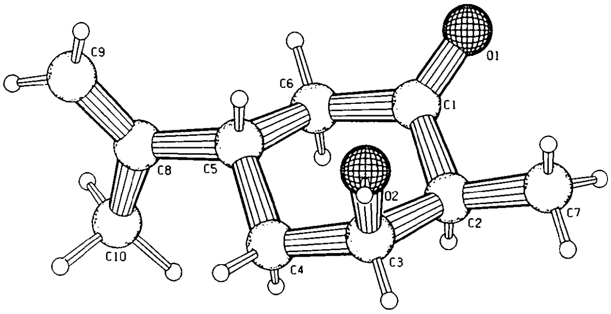

Fig. 1. View of the molecule with atom numbering.

Table 2. *Bond lengths* (Å) *and bond angles* (°)

O(1)—C(1)	1·224 (3)	C(3)—C(4)	1·514 (3)
O(2)—C(3)	1·438 (2)	C(4)—C(5)	1·535 (3)
C(1)—C(2)	1·507 (3)	C(5)—C(6)	1·536 (3)
C(1)—C(6)	1·508 (3)	C(5)—C(8)	1·512 (3)
C(2)—C(3)	1·543 (3)	C(8)—C(9)	1·345 (4)
C(2)—C(7)	1·506 (4)	C(8)—C(10)	1·472 (4)
O(1)—C(1)—C(2)	122·4 (2)	C(3)—C(4)—C(5)	111·7 (2)
O(1)—C(1)—C(6)	121·5 (2)	C(4)—C(5)—C(6)	109·3 (2)
C(2)—C(1)—C(6)	116·0 (2)	C(4)—C(5)—C(8)	114·2 (2)
C(1)—C(2)—C(3)	111·0 (2)	C(6)—C(5)—C(8)	110·6 (2)
C(1)—C(2)—C(7)	113·2 (2)	C(1)—C(6)—C(5)	111·7 (2)
C(3)—C(2)—C(7)	113·5 (2)	C(5)—C(8)—C(9)	120·0 (3)
O(2)—C(3)—C(2)	108·2 (2)	C(5)—C(8)—C(10)	118·0 (2)
O(2)—C(3)—C(4)	110·4 (2)	C(9)—C(8)—C(10)	122·0 (2)
C(2)—C(3)—C(4)	112·2 (2)		

assembled in Table 2. The cyclohexanone ring exhibits a chair conformation (Boeyens, 1978) with puckering parameters $Q = 0{\cdot}543$ (2) Å, $\theta = 7{\cdot}9$ (2) and $\varphi = 205$ (2)° (Cremer & Pople, 1975). The methyl group assumes an equatorial position, making an angle of 71·1 (2)° with the normal to the Cremer & Pople plane. The molecules are linked *via* a hydrogen bond [O(2)—H(1)···O(1), with O(2)···O(1) = 2·892 (2), O(2)—H(1) = 0·74 (3), H(1)···O(1) = 2·200 (3) Å and O(2)—H(1)···O(1) = 156 (3)°] into an infinite chain running in the *a*-axis direction.

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Structure of α-D-Mannosido-naphtho-18-crown-6:* A Potent Host for Chiral Recognition

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Abstract. (Methyl 2,3-dideoxy-4,6-*O*-isopropylidenemannopyranosido)-naphtho-18-crown-6, $C_{28}H_{38}O_{10}$, $M_r = 534{\cdot}6$, monoclinic $P2_1$, $a = 11{\cdot}606$ (2), $b = 8{\cdot}126$ (4), $c = 14{\cdot}977$ (2) Å, $\beta = 102{\cdot}38$ (2)°, $V = 1379$ (2) Å^3, $Z = 2$, $D_x = 1{\cdot}287$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, $\mu = 0{\cdot}909$ cm^{-1}, $F(000) = 572$, $T = 298$ K, final $R = 0{\cdot}035$ for 2108 reflections. In its

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* IUPAC name: methyl 4,6-*O*-isopropylidene-2,3-*O*-{2,3-naphthylenebis(oxyethyleneoxyethylene)}mannopyranoside.

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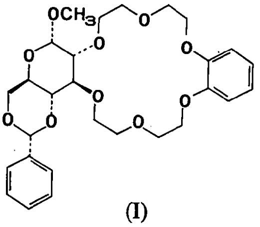
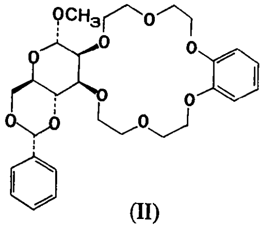
uncomplexed form the 18-crown-6 macrocyclic ring of the ligand has a highly distorted conformation stabilized by three short C—H···O intramolecular contacts 'across' the internal cavity.

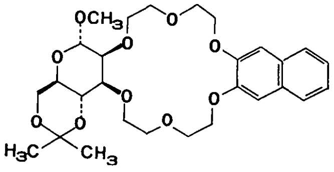
Introduction. Chiral crown polyethers are potent host molecules for selective recognition of enantiomers such as amino acids and their derivatives (Géhin, Di Cesare & Gross, 1986). Crystal structures of chirally substituted 18-crown-6 where the chiral substituent is a sugar derivative have been reported up to now only for complexed ligands such as α-D-glucosido-benzo-18-crown-6 (I) with: KI (Suwińska, Pietraszkiewicz, Lipkowski, Jurczak, Andreetti & Bocelli, 1981), KSCN (Suwińska & Andreetti, 1983), (*R*)-phenylglycine methyl ester hexafluorophsphate (Courtois, El Masdouri, Géhin & Gross, 1986) and α-D-mannosido-benzo-18-crown-6 (II) with KSCN (Suwińska & Lipkowski, 1988). For the first time the structure of the 'free' ligand α-D-mannosido-naphtho-18-crown-6 (III) is presented, thus allowing for comparison between the complexed and uncomplexed forms of the ligand.



(I)



(II)



(III)

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and isotropic thermal parameters* (Å^2) *for non*-H *atoms with e.s.d.'s in parentheses*

	x	*y*	*z*	B_{eq}*
C(1)	7975 (3)	311 (6)	13027 (2)	5·89 (9)
C(2)	9295 (3)	2268 (5)	12427 (2)	5·66 (9)
C(3)	8109 (3)	1413†	12246 (2)	4·20 (7)
O(4)	7161 (2)	2572 (3)	12148 (1)	5·17 (5)
C(5)	6966 (3)	3554 (4)	11335 (2)	5·16 (8)
C(6)	6774 (3)	2389 (4)	10526 (2)	4·24 (7)
C(7)	7836 (3)	1264 (4)	10612 (2)	3·66 (6)
O(8)	7947 (2)	371 (3)	11456 (1)	3·90 (4)
O(9)	6657 (2)	3375 (3)	9717 (1)	4·46 (5)
C(10)	6433 (3)	2375 (4)	8916 (2)	4·32 (7)
C(11)	7370 (2)	1072 (4)	8927 (2)	3·81 (6)
C(12)	7624 (2)	70 (4)	9817 (2)	3·60 (6)
O(13)	5334 (2)	1588 (3)	8793 (2)	5·11 (6)
C(14)	4388 (3)	2734 (6)	8603 (3)	7·6 (1)
O(15)	8402 (2)	1954 (3)	8827 (1)	4·38 (5)
C(16)	9036 (3)	1246 (5)	8221 (2)	4·64 (7)
C(17)	9649 (3)	2626 (5)	7827 (2)	5·58 (9)
O(18)	8800 (2)	3667 (3)	7212 (2)	5·58 (6)
C(19)	8498 (3)	3059 (6)	6326 (2)	5·68 (8)
C(20)	7178 (3)	3226 (5)	5971 (2)	4·53 (7)
O(21)	6632 (2)	1952 (3)	6400 (1)	4·41 (5)
C(22)	5435 (2)	1791 (4)	6152 (2)	3·61 (6)
C(23)	4684 (3)	2845 (4)	5611 (2)	4·15 (7)
C(24)	3440 (3)	2560 (4)	5425 (2)	3·89 (6)
C(25)	2637 (3)	3599 (5)	4847 (2)	4·88 (8)
C(26)	1450 (3)	3308 (5)	4685 (2)	5·47 (9)
C(27)	1014 (3)	1977 (6)	5094 (2)	5·71 (9)
C(28)	1765 (3)	926 (5)	5657 (2)	4·93 (8)
C(29)	3008 (2)	1174 (4)	5829 (2)	3·87 (6)
C(30)	3807 (2)	83 (4)	6362 (2)	3·87 (6)
C(31)	4992 (2)	332 (4)	6505 (2)	3·66 (6)
O(32)	5847 (2)	−697 (3)	6956 (1)	4·14 (5)
C(33)	5478 (3)	−2331 (4)	7145 (2)	4·92 (8)
C(34)	6574 (3)	−3262 (4)	7556 (2)	4·67 (7)
O(35)	6953 (2)	−2746 (3)	8475 (1)	4·44 (5)
C(36)	8103 (3)	−3337 (4)	8884 (2)	4·50 (7)
C(37)	8464 (3)	−2665 (4)	9837 (2)	4·83 (8)
O(38)	8649 (2)	−924 (3)	9861 (1)	4·18 (5)

* $B_{eq} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta) \times B(1,3) + bc(\cos\alpha)B(2,3)]$.

† Origin-defining.

Experimental. Crystal approximate dimensions 0·35 × 0·35 × 0·52 mm; intensities measured at 298 K on Enraf–Nonius CAD-4 four-circle diffractometer (Mo *Kα* radiation, graphite monochromator). Lattice parameters determined by least squares from 23 reflections ($5 < \theta < 11°$). Total of 2893 reflections up to $\theta = 25°$ ($0 \leq h \leq 13$, $0 \leq k \leq 9$, $-17 \leq l \leq 17$) measured in the ω–2θ scan mode; 2610 unique reflections ($R_{int} = 0·011$), 2108 reflections considered as observed [$F_o > 2\sigma(F_o)$]. The intensity variation of three standard reflections, measured every hour, was less than 1%. No absorption or secondary-extinction correction. Structure solved by *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and refined by full-matrix least squares with the *SDP* system (B.A. Frenz & Associates, Inc., 1985). Weights of each reflection in refinement (on *F*) calculated from $w = 1/\sigma^2(F_o)$, $\sigma(F_o)$ being the e.s.d., based on counting statistics, of the observed structure factor. Scattering factors taken from *International Tables for X-ray Crystallography* (1974). All H atoms included in the refinement in calculated positions [d(C—H) = 1·08 Å]. The total number of parameters refined was 342: one scale factor, position parameters and anisotropic thermal parameters for non-H atoms; no attempt was made to refine the positions or isotropic thermal parameters for H atoms. Refinement resulted in final values of $R = 0·035$, $wR = 0·034$ and $S = 2·86$; in the last cycle $(\Delta/\sigma)_{max} = 0·03$. Final max. and min. $\Delta\rho$ were 0·24 and $-0·13$ e Å^{-3}, respectively. All calculations performed on a MicroPDP11/73 computer. The final atomic coordinates are given in Table 1.*

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* Lists of structure factors, anisotropic thermal parameters for the non-H atoms, positional and isotropic thermal parameters for the H atoms and a table of the shortest non-bonded contacts have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52450 (29 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Selected bond distances* (Å) *and angles* (°) *for non*-H *atoms with e.s.d.'s in parentheses*

C(1)—C(3)	1·508 (5)	O(13)—C(14)	1·422 (4)
C(2)—C(3)	1·513 (4)	O(15)—C(16)	1·408 (4)
C(3)—O(4)	1·431 (4)	C(16)—C(17)	1·514 (5)
C(3)—O(8)	1·434 (3)	C(17)—O(18)	1·465 (4)
O(4)—C(5)	1·432 (4)	O(18)—C(19)	1·388 (4)
C(5)—C(6)	1·516 (4)	C(19)—C(20)	1·516 (5)
C(6)—C(7)	1·517 (4)	C(20)—O(21)	1·436 (4)
C(6)—O(9)	1·434 (4)	O(21)—C(22)	1·366 (3)
C(7)—O(8)	1·439 (3)	C(22)—C(31)	1·436 (4)
C(7)—C(12)	1·514 (5)	C(31)—O(32)	1·361 (3)
O(9)—C(10)	1·425 (4)	O(32)—C(33)	1·442 (4)
C(10)—C(11)	1·515 (4)	C(33)—C(34)	1·494 (4)
C(10)—O(13)	1·403 (4)	C(34)—O(35)	1·415 (3)
C(11)—C(12)	1·537 (5)	O(35)—C(36)	1·427 (3)
C(11)—O(15)	1·432 (4)	C(36)—C(37)	1·502 (4)
C(12)—O(38)	1·427 (3)	C(37)—O(38)	1·430 (4)
C(3)—O(4)—C(5)	115·6 (2)	C(10)—O(13)—C(14)	111·6 (3)
O(4)—C(5)—C(6)	107·5 (3)	C(11)—O(15)—C(16)	115·3 (2)
C(5)—C(6)—C(7)	109·3 (2)	O(15)—C(16)—C(17)	107·6 (3)
C(5)—C(6)—O(9)	107·4 (3)	C(16)—C(17)—O(18)	111·3 (2)
C(7)—C(6)—O(9)	109·7 (2)	C(17)—O(18)—C(19)	113·2 (3)
C(6)—C(7)—O(8)	107·3 (2)	O(18)—C(19)—C(20)	109·4 (3)
C(6)—C(7)—C(12)	109·1 (3)	C(19)—C(20)—O(21)	106·7 (3)
O(8)—C(7)—C(12)	109·6 (2)	C(20)—O(21)—C(22)	118·0 (2)
C(3)—O(8)—C(7)	113·5 (2)	O(21)—C(22)—C(23)	125·9 (3)
C(6)—O(9)—C(10)	111·1 (2)	O(21)—C(22)—C(31)	113·7 (2)
O(9)—C(10)—C(11)	112·9 (2)	C(22)—C(31)—O(32)	114·2 (2)
O(9)—C(10)—O(13)	111·5 (3)	C(30)—C(31)—O(32)	126·2 (3)
C(11)—C(10)—O(13)	108·2 (3)	C(31)—O(32)—C(33)	116·6 (2)
C(10)—C(11)—C(12)	112·5 (3)	O(32)—C(33)—C(34)	106·6 (2)
C(10)—C(11)—O(15)	105·3 (3)	C(33)—C(34)—O(35)	108·0 (3)
C(12)—C(11)—O(15)	110·3 (2)	C(34)—O(35)—C(36)	112·6 (2)
C(7)—C(12)—C(11)	108·1 (3)	O(35)—C(36)—C(37)	109·3 (3)
C(7)—C(12)—O(38)	109·5 (2)	C(36)—C(37)—O(38)	113·2 (3)
C(11)—C(12)—O(38)	110·1 (2)	C(12)—O(38)—C(37)	116·1 (2)

Table 3. *Torsion angles* (°) *in the macrocyclic* 18-*membered ring with e.s.d.'s in parentheses*

C(12)—C(11)—O(15)—C(16)	101·2 (3)	−169·6 (8)*
C(11)—O(15)—C(16)—C(17)	151·4 (2)	−178·4 (8)
O(15)—C(16)—C(17)—O(18)	−69·2 (3)	−80·9 (6)
C(16)—C(17)—O(18)—C(19)	−84·8 (3)	167·8 (8)
C(17)—O(18)—C(19)—C(20)	137·0 (3)	171·1 (8)
O(18)—C(19)—C(20)—O(21)	−75·8 (4)	65·6 (6)
C(19)—C(20)—O(21)—C(22)	−176·6 (2)	−174·9 (8)
C(20) -O(21)—C(22)—C(31)	170·6 (2)	166·2 (9)
O(21)—C(22)—C(31)—O(32)	−5·3 (3)	6·7 (6)
C(22)—C(31)—O(32)—C(33)	−166·5 (3)	179·6 (9)
C(31)—O(32)—C(33)—C(34)	174·6 (2)	−171·2 (8)
O(32)—C(33)—C(34)—O(35)	76·4 (3)	−65·7 (6)
C(33)—C(34)—O(35)—C(36)	−169·5 (2)	−172·7 (9)
C(34)—O(35)—C(36)—C(37)	177·0 (3)	−172·7 (10)
O(35)—C(36)—C(37)—O(38)	−67·6 (3)	60·3 (7)
C(36)—C(37)—O(38)—C(12)	85·0 (3)	152·9 (9)
C(11)—C(12)—O(38)—C(37)	−114·6 (3)	−133·2 (8)
O(15)—C(11)—C(12)—O(38)	−52·3 (3)	54·9 (5)

* Data for the complex of (II) with KSCN (Suwińska & Lipkowski, 1988).

Discussion. Bond distances and angles are given in Table 2, torsion angles in the macrocylic ring are listed in Table 3. The numbering scheme is shown in Fig. 1. The bond lengths and bond angles in the aromatic naphthalene moiety are similar to those found for the naphthalene molecule at 239 K (Brock & Dunitz, 1982) [range from 1·359 (4) to 1·436 (4) Å for the bond distances and from 118·1 (3) to 122·3 (4)° for the bond angles]. The $C(sp^3)$—O [1·388 (4)–1·465 (4), average 1·428 Å] and $C(sp^3)$—$C(sp^3)$ [1·494 (4)–1·537 (5) average 1·513 Å] distances in the macrocyclic ring follow the trends usual for crown ether compounds (Dunitz & Seiler, 1974). $C(sp^3)$—$C(sp^3)$—O angles in the macrocyclic ring vary from 106·6 (2) to 113·2 (3)° (average 109·3°); $C(sp^3)$—O—$C(sp^3)$ bond angles may be classified in two groups: angles at O(18) and O(35) equal to 113·2 (3) and 112·6 (2)°, respectively, and at O(15), O(21), O(32) and O(38) which are larger by about 3° [range 115·3 (2)–118·0 (2), average 116·5°]. The same tendency was observed in other macrocyclic ligands bearing chiral sugar substituents derived from glucose and mannose (Suwińska *et al.*, 1981; Suwińska

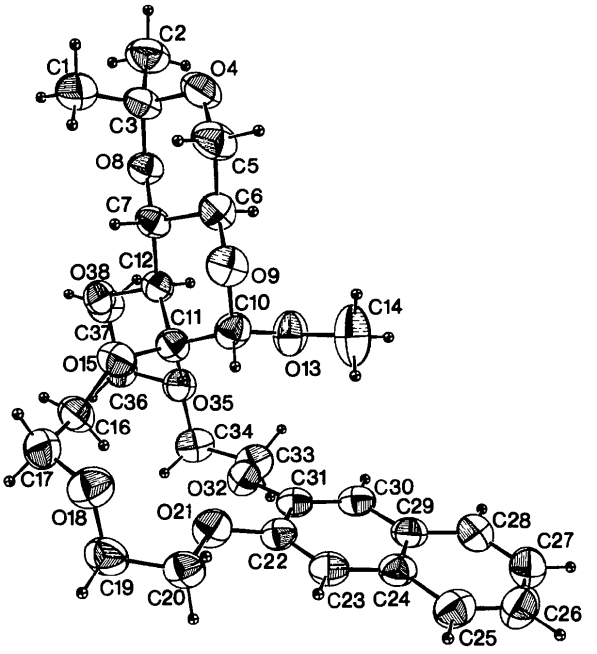

Fig. 1. *ORTEP*II (Johnson, 1976) view of the molecule with the atom numbering. The thermal ellipsoids are given at 50% probability.

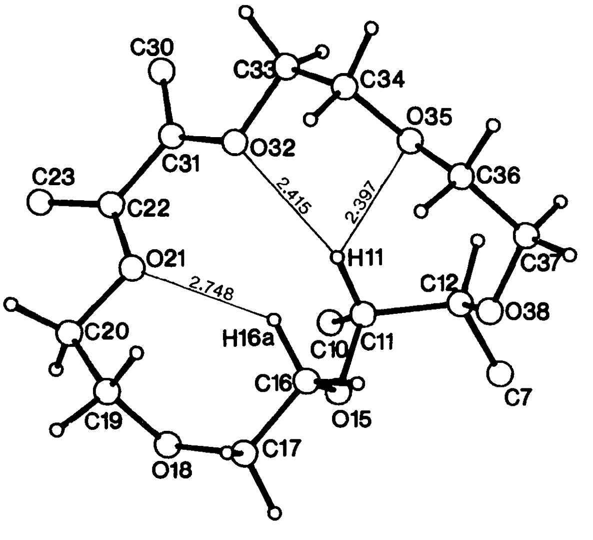

Fig. 2. The conformation of the macrocyclic ring showing the short intramolecular contacts.

& Andreetti, 1983; Courtois *et al.*, 1986; Suwińska & Lipkowski, 1988). The conformation of the macrocyclic ring is described by torsion angles (Table 3). The sequence of dihedral angles along the macrocylic ring is $g^+ag^-g^-ag^-aa0aag^+aag^-g^+g^-g^-$ and is different from that for the complex of α-D-mannosido-benzo-18-crown-6 (II) with KSCN (Suwińska & Lipkowski, 1988) which was much closer to the 'ideal' conformation with energetically preferred *gauche* (*g*) conformation about C—C bonds and anti (*a*) about C—O bonds. The *gauche* conformation about C(11)—O(15), C(17)—O(18), C(37)—O(38) and C(12)—O(38) bonds forces the macrocyclic ring into a highly distorted conformation, minimizing the size of the molecular cavity. The cavity, which in complexed form contains the K^+ cation, in the present structure contains H atoms H(11) and H(16*a*) which are pointing towards the center of the macrocyclic cavity, giving short intramolecular contacts 'across' the ring (Fig. 2). The O(21) and O(32) atoms are out of the plane of the naphthalene rings by −0·082 (2) and +0·183 (2) Å, respectively. The four O atoms of the macrocyclic ring, O(18), O(21), O(32) and O(35), are coplanar to within 0·022 (2) Å; the remaining two O atoms deviate from that plane by −1·299 (2) Å [O(15)] and −1·019 (2) Å [O(38)].

The shortest interatomic distances between non-H atoms of adjacent different molecules are: no C···C or O···O below 3·5 Å, O···C 3·389 (4) Å between O(4) and C(30) at $1-x, \frac{1}{2}+y, 2-z$.

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1-Phosphabicyclo[3.3.0]octane 1-Sulfide

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Abstract. $C_7H_{13}PS$, $M_r = 160·2$, monoclinic, $P2_1/c$, $a = 7·647\ (1)$, $b = 7·841\ (1)$, $c = 14·508\ (4)$ Å, $\beta = 99·96\ (3)°$, $V = 856·8\ (3)$ Å^3, $Z = 4$, $D_x = 1·24$ Mg m^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1·5418$ Å, $\mu = 4·43$ mm^{-1}, $F(000) = 344$, $T = 291$ K, final $R = 0·056$ for 981 observed reflections. The phospholane rings of the 1-phosphabicyclo[3.3.0]octane 1-sulfide molecule are *cis*-fused and both adopt an envelope conformation. In one ring the flap C atom is positionally disordered. As a result of this disorder, the title compound exists in both an *exo–endo* conformation (main occupancy) and an *endo–endo* conformation in the solid state.

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