C34—C2—C24—C25	176.9 (2)	C14—C4—C44—C45	84.3 (3)
C24—C2—C34—C35	−100.4 (3)	C44—C4—C14—C15	−161.5 (2)
C42—C3—C32—C31	93.0 (2)	C22—C1—C12—C11	−96.4 (2)
C32—C3—C42—C41	−86.2 (2)	C12—C1—C22—C21	85.2 (2)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O5'	0.82	1.88	2.677 (2)	165
O2—H2···O1	0.82	1.93	2.742 (2)	171
O3—H3···O6	0.82	1.83	2.618 (3)	162
O4—H4···O3	0.82	1.87	2.681 (2)	171
O5—H5···O4	0.82	1.93	2.724 (2)	164
O6—H6···O2^{ii}	0.82	1.90	2.702 (2)	165

Symmetry codes: (i) $x, y-1, z$; (ii) $x, 1+y, z$.

The calix[4]arene lies in a general position in the cell and it soon became apparent that there were also two independent methanol molecules in the asymmetric unit. All H atoms were visible in difference maps and were allowed for as riding atoms using appropriate *AFIX* controls in the *SHELXL*93 (Sheldrick, 1993) refinement, with C—H 0.93–0.97 and O—H 0.82 Å.

Data collection: *CAD-4-PC* (Enraf–Nonius, 1992). Cell refinement: *SET*4 and *CELDIM CAD-4-PC*. Data reduction: *DATRD*2 in *NRCVAX*96 (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *NRCVAX*96 and *SHELXL*93). Molecular graphics: *NRCVAX*96, *ORTEP*II (Johnson, 1976), *PLATON* (Spek, 1996*a*) and *PLUTON* (Spek 1996*b*). Software used to prepare material for publication: *NRCVAX*96, *SHELXL*93 and WordPerfect macro *PREPCIF*97 (Ferguson, 1997).

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Trimethoprim–Sulfadimidine 1:2 Molecular Complex Monohydrate

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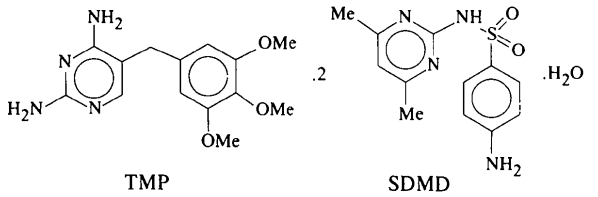
Abstract

In the title compound, $C_{14}H_{18}N_4O_3.2C_{12}H_{14}N_4O_2S.H_2O$, trimethoprim [5-(3,4,5-trimethoxybenzyl)pyrimidine-2,4-diamine, TMP] interacts with one sulfadimidine [4-amino-*N*-(4,6-dimethyl-2-pyrimidinyl)benzenesulfonamide, SDMD] molecule through two N—H···N hydrogen bonds forming an eight-membered ring, as in the 1:1 methanolate complex, with no proton transfer from the imino sulfonamide N atom to the pyrimidine N atom of the partner. Association with the second sulfadimidine molecule (SDMD′) occurs through an N—H···N interaction involving the same pyrimidine N atom of TMP (which therefore acts as a double acceptor) and the NH imino group of the sulfonamide. The water molecule bridges the sulfonamido O atom and the *p*-aminophenyl group of SDMD′ of two molecular complex units.

Comment

The previous paper on a 1:1 TMP–SDMD complex methanol solvate indicated (*a*) the absence of TMP protonation by the sulfonamide partner, unlike in the TMP complexes with sulfametrole and sulfamethoxazole, and (*b*) the very strong interaction between the methanol and the sulfonyl group without a direct contribution to crystal packing from the solvent (Bettinetti & Sardone, 1997). Since, in aqueous ethanolic solution, TMP and SDMD form a 1:2 molecular complex, the present study was undertaken to elucidate the nature of molecular association between TMP and SDMD in water

and to compare the structural features in different solvated forms of the same complexed species. In the title complex (Fig. 1), TMP is associated with the sulfadimidine molecule SDMD through two non-ionic N—H···N interactions [HN1···N7 2.14 Å, N1—HN1···N7 171° and N1···N7 2.991 (3) Å; HN6*B*···N2 2.16 Å, N6—HN6*B*···N2 160° and N6···N2 3.140 (3) Å] forming the same eight-membered ring arrangement reported by Bettinetti & Sardone (1997).



TMP SDMD

The absence of TMP protonation is confirmed by the value of the C13—N7—C14 angle [115.0 (2)°] (Singh, 1965), which is very similar to that in free TMP (Koetzle & Williams, 1976). TMP protonation however occurs in its complexes with sulfametrole (Giuseppetti, Tadini & Bettinetti, 1994) and sulfamethoxazole (Nakai, Takasuka & Shiro, 1984). This supports our earlier observations that the acid strength displayed in aqueous media by SDMD (pK_a 7.4), sulfamethoxazole (pK_a 5.7) and sulfametrole (pK_a 4.8) is reflected in the nature of the respective solid-state interactions with TMP. It should be noted that sulfadimidine is able to protonate its partner in the solid-state complex with aminacrine (Ghose, Chakrabarti, Dattagupta, Le Page & Trotter, 1988), which is a stronger base than TMP. Deprotonation of SDMD does not obviously occur with partners of acidic character such as 4-aminosalicylic acid (Caira, 1992), 2-aminobenzoic acid (Caira, 1991) and salicylic acid (Patel, Haridas & Singh, 1988). Both sulfadimidine molecules in the present complex are in the amido tautomeric form, with N—C and N—S sulfonamide bond distances in the expected range for the protonated species. If one compares the TMP and SDMD molecules forming the eight-membered ring arrangement in the title compound with those in the 1:1 methanol solvated complex (Bettinetti & Sardone, 1997), the major differences occur in the N···N hydrogen bonds distances (longer by 0.2–0.1 Å in the present complex), in the respective conformations and in the relative orientation of the pyrimidine and phenyl planes. In particular, in TMP, the conformational parameters τ_1(TMP) (C16—C15—C17—C18) and τ_2(TMP) (C15—C17—C18—C26), and the angle between the diaminopyrimidine and trimethoxybenzyl

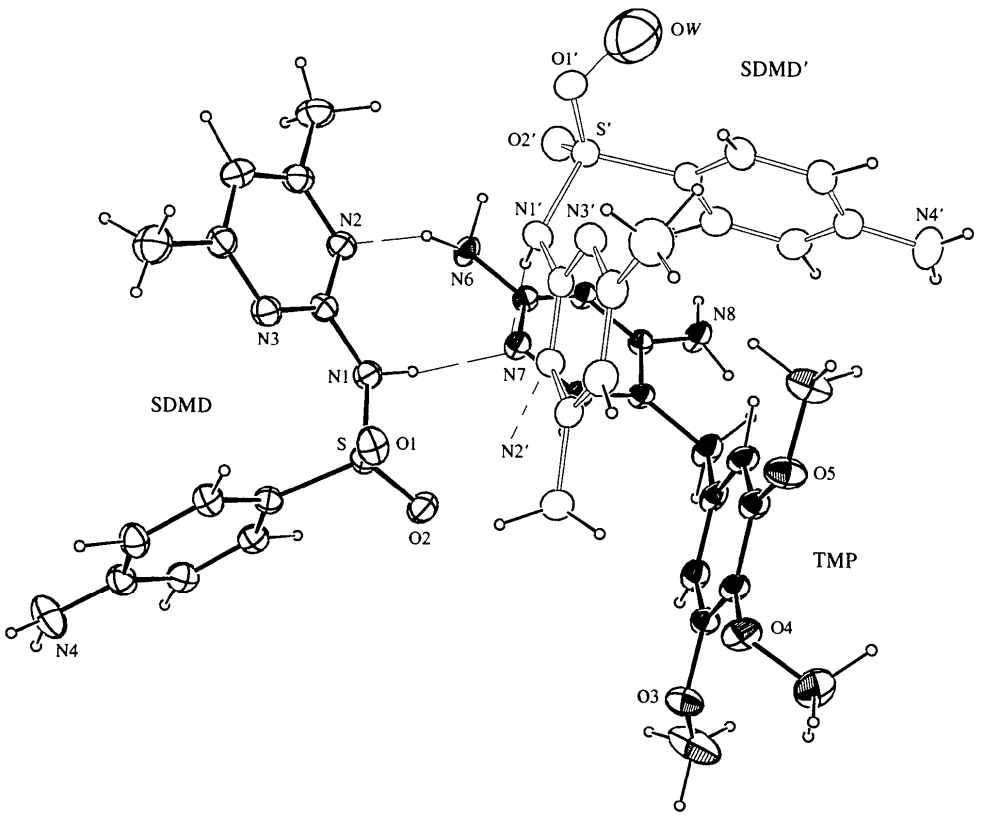


Fig. 1. Perspective view of the complex with 30% probability displacement ellipsoids.

rings are 166.7 (3), −76.1 (4) and 82.8 (1)°, respectively, in the present structure. The corresponding angles are −88.3 (3), 158.3 (2) and 104.6 (6)°, respectively, in the 1:1 complex. Hence, the conformation adopted here is different from that found in the 1:1 complex and resembles that of the TMP cation in TMP hydrochloride [τ_1(TMP) = 156.4 (1) and τ_2(TMP) = 62.5 (2)°] and the TMP–sulfamethoxazole complex [τ_1(TMP) = −172.9 (3) and τ_2(TMP) = 90.6 (4)°] (Nakai, Takasuka & Shiro, 1984).

The major difference in conformational parameters between sulfadimidine involved in the eight-membered ring in the 1:2 complex [τ_1(SDMD) (N1—S—C7—C8) = 78.8 (3), τ_2(SDMD) (C7—S—N1—C1) = 68.5 (3) and τ_3(SDMD) (S—N1—C1—N3) = −8.0 (4)°, and the angle between the dimethylpyrimidine and *p*-aminophenyl rings is 107.8 (1)°] and the 1:1 methanol solvate complex [respective values 131.2 (2), −65.2 (2), 10.5 (2) and 92.2 (1)°] occurs in torsion angle τ_1 which is reported to range between 70–120° in the sulfadimidine rotamers (Caira, 1992). The SDMD′ molecule is linked to the same basic N7 atom of TMP (which therefore acts as a double acceptor) as SDMD, through an N—H···N interaction [HN1′···N7 2.36, N1′···N7 3.218 (4) Å and N1′—HN1′···N7 168°] which is almost perpendicular to the eight-membered ring plane. It displays intramolecular bond distances and angles similar to those observed in SDMD, but differences in conformational parameters [τ_1(SDMD′) = −97.7 (2), τ_2(SDMD′) = 48.1 (3) and τ_3(SDMD′) = 35.0 (4)°, and the angle between the dimethylpyrimidine and *p*-aminophenyl rings is 72.3 (1)°] illustrate the observed conformational flexibility of this sulfonamide (Rambaud *et al.*, 1985). The water molecule bridges the SDMD′ molecules of two complex units acting as donor toward the sulfonamido O1′ atom [*OW*···O1′ 2.861 (2) Å; water H atoms were not found in the difference Fourier map and so were disregarded] and as acceptor toward the *p*-aminophenyl group of a symmetry-related molecule [HN4*B*′···*OW* 2.252 (2), N4′···*OW*^{i} 3.066 (5) Å and N4′—HN4*B*′···*OW*^{i} 155°]. The solvent, thus plays an important role in the stabilization of the crystal structure. This feature is reflected in the thermal behaviour of the title compound, specifically by water leaving the crystal lattice at the melting point, *i.e.* about 433 K under the standard experimental conditions of differential scanning calorimetry and thermogravimetry (heating rate 10 K min^{-1} in the 303–473 K temperature range in an open pan under static air). The solvent evolution from the crystal lattice of the methanol solvate complex, where methanol is involved in a unique O···O interaction [2.931 (3) Å] with a sulfonamido O atom, occurs at a relatively lower temperature (419 K) under the same experimental conditions (Bettinetti & Sardone, 1997).

Besides the van der Waals interactions, the crystal packing is stabilized by a wide hydrogen-bonding network in which all the acidic H atoms participate as shown in Fig. 2: HN4*A*···O2^{ii} 2.15, N4···O2^{ii} 3.214 (4) Å and N4—HN4*A*···O2^{ii} 169°; N4—HN4*B*···O3^{ii} 179°, HN4*B*···O3^{ii} 2.16 and N4···O3^{ii} 3.104 (4) Å; N6···O2′^{iii} 3.231 (3), HN6*A*···O2′^{iii} 2.28 Å and N6—HN6*A*···O2′^{iii} 148°; N8···N5^{iv}

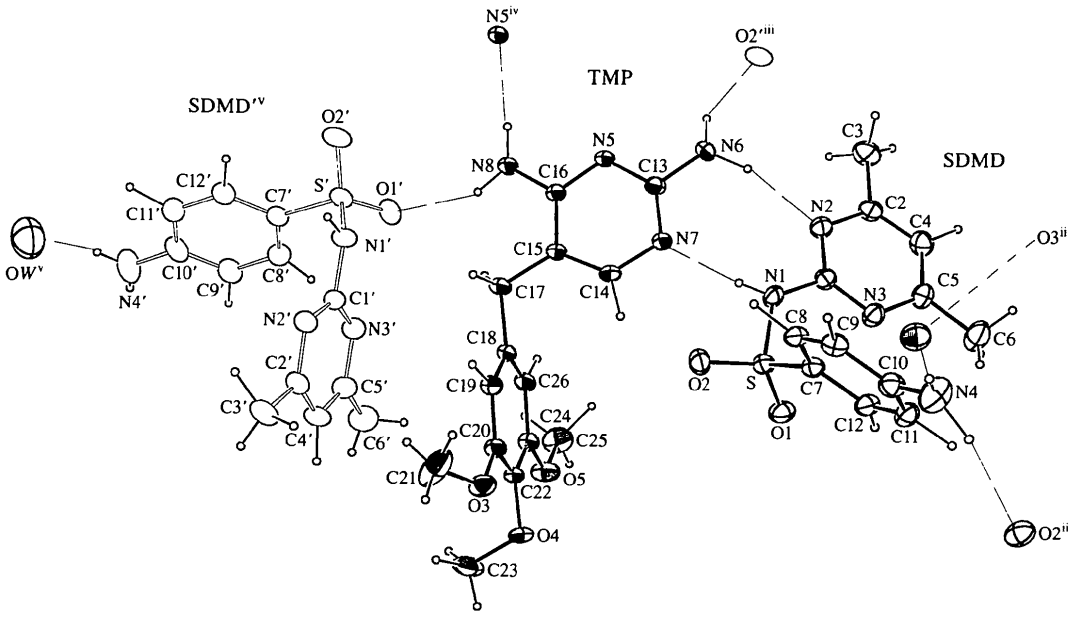


Fig. 2. View of the principal hydrogen-bonding interactions in the crystal. The SDMD′ and water molecules are translated by one unit along the *b* axis for clarity. C atoms are labelled with numerals only. Symmetry codes: (i) x, $1+y$, z; (ii) $-\frac{1}{2}-x$, $y-\frac{3}{2}$, $-\frac{1}{2}-z$; (iii) $-x$, $-y$, $-z$; (iv) $-x$, $1-y$, $-z$.

3.083 (3), HN8*A*···N5^{iv} 2.14 Å and N8—HN8*A*···N5^{iv} 168°; N8···O1$'^{v}$ 3.016 (3), HN8*B*···O1$'^{v}$ 2.25 Å and N8—HN8*B*···O1$'^{v}$ 140°; symmetry codes: (i) x, $1+y$, z; (ii) $-\frac{1}{2}-x$, $y-\frac{3}{2}$, $-\frac{1}{2}-z$; (iii) $-x$, $-y$, $-z$; (iv) $-x$, $1-y$, $-z$.

Experimental

Single crystals of the title compound were prepared by recrystallization of 1.45 g (0.005 mol) TMP and 2.78 g (0.01 mol) SDMD from 50 ml of 50:50 ethanol–water.

Crystal data

$C_{14}H_{18}N_4O_3.2C_{12}H_{14}N_4O_2S.H_2O$
M_r = 864.99
Monoclinic
$P2_1/n$
a = 11.075 (1) Å
b = 9.268 (1) Å
c = 40.170 (5) Å
β = 94.05 (1)°
V = 4112.9 (8) Å^3
Z = 4.00
D_x = 1.3969 Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
λ = 1.54184 Å
Cell parameters from 25 reflections
θ = 30–34°
μ = 1.6942 mm^{-1}
T = 293 (3) K
Prism
0.58 × 0.50 × 0.18 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North, Phillips & Mathews, 1968)
T_{min} = 0.576, T_{max} = 0.737
8827 measured reflections
7339 independent reflections

6251 reflections with $I > 3\sigma(I)$
R_{int} = 0.01
θ_{max} = 70°
$h = -13 \rightarrow 13$
$k = -1 \rightarrow 11$
$l = 0 \rightarrow 49$
3 standard reflections
every 300 reflections
intensity decay: 3.2%

Refinement

Refinement on F
R = 0.049
wR = 0.050
S = 1.616
7339 reflections
542 parameters
H atoms not refined
Unit weights applied
$(\Delta/\sigma)_{max}$ = 0.02

$\Delta\rho_{max}$ = 0.297 e Å^{-3}
$\Delta\rho_{min}$ = −0.137 e Å^{-3}
Extinction correction: Zachariasen (1963)
Extinction coefficient: 7.9264 × 10
Scattering factors from *International Tables for X-ray Crystallography* (Vol. IV)

Table 1. *Selected geometric parameters (Å, °)*

S—O1	1.425 (2)	N1′—C1′	1.406 (4)
S—O2	1.441 (2)	N3′—C1′	1.332 (4)
S—N1	1.647 (2)	N3′—C5′	1.351 (4)
S—C7	1.744 (3)	N2′—C1′	1.325 (4)
N1—C1	1.383 (4)	N2′—C2′	1.344 (4)
N2—C1	1.332 (4)	N4′—C10′	1.374 (5)
N2—C2	1.347 (4)	C5′—C6′	1.502 (5)
N3—C1	1.331 (4)	C5′—C4′	1.375 (5)
N3—C5	1.343 (4)	C4′—C2′	1.379 (5)
N4—C10	1.369 (4)	C2′—C3′	1.491 (5)
C2—C3	1.491 (4)	N5—C13	1.343 (4)
C2—C4	1.380 (5)	N5—C16	1.346 (4)
C4—C5	1.380 (5)	N6—C13	1.374 (4)
C5—C6	1.488 (5)	N7—C13	1.333 (3)
S′—O1′	1.436 (2)	N7—C14	1.367 (4)
S′—O2′	1.434 (2)	N8—C16	1.342 (4)
S′—N1′	1.649 (2)	C14—C15	1.358 (4)
S′—C7′	1.741 (3)	C15—C16	1.421 (4)
N1—S—C7	107.0 (1)	S′—N1′—C1′	123.2 (2)
O2—S—C7	108.9 (1)	C1′—N3′—C5′	114.5 (3)
O2—S—N1	102.9 (1)	C1′—N2′—C2′	115.6 (3)
O1—S—C7	107.4 (1)	N3′—C1′—N2′	128.9 (3)
O1—S—N1	111.3 (1)	N1′—C1′—N2′	113.8 (2)
O1—S—O2	118.8 (1)	N1′—C1′—N3′	117.3 (3)
S—N1—C1	124.5 (2)	N3′—C5′—C4′	121.3 (3)
C1—N2—C2	115.7 (3)	N3′—C5′—C6′	116.2 (3)
C1—N3—C5	116.2 (3)	C6′—C5′—C4′	122.4 (3)
N2—C1—N3	127.6 (3)	C5′—C4′—C2′	119.1 (3)
N1—C1—N3	117.4 (3)	N2′—C2′—C4′	120.6 (3)
N1—C1—N2	115.0 (3)	C4′—C2′—C3′	121.9 (3)
N2—C2—C4	120.9 (3)	N2′—C2′—C3′	117.5 (3)
N2—C2—C3	116.1 (3)	S′—C7′—C12′	118.5 (2)
C3—C2—C4	123.0 (3)	S′—C7′—C8′	121.2 (3)
C2—C4—C5	118.9 (3)	C8′—C7′—C12′	120.3 (3)
N3—C5—C4	120.7 (3)	N4′—C10′—C11′	120.5 (3)
C4—C5—C6	123.0 (3)	N4′—C10′—C9′	119.9 (3)
N3—C5—C6	116.3 (3)	C13—N5—C16	116.6 (2)
S—C7—C12	119.3 (2)	C13—N7—C14	115.0 (2)
S—C7—C8	120.5 (2)	N6—C13—N7	116.8 (3)
N4—C10—C9	121.8 (3)	N5—C13—N7	126.7 (3)
N4—C10—C11	119.2 (3)	N5—C13—N6	116.4 (2)
N1′—S′—C7′	106.1 (1)	N7—C14—C15	124.4 (2)
O2′—S′—C7′	110.3 (2)	C14—C15—C16	115.4 (3)
O2′—S′—N1′	103.9 (1)	N8—C16—C15	121.7 (3)
O1′—S′—C7′	108.8 (1)	N5—C16—C15	121.9 (3)
O1′—S′—N1′	109.0 (1)	N5—C16—N8	116.3 (2)
O1′—S′—O2′	117.9 (1)		

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CELDIM* in *CAD-4 Software*. Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *MULTAN*80 (Main *et al.*, 1980). Program(s) used to refine structure: *MolEN*. Molecular graphics: *ORTEP*II (Johnson 1976). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1044). Services for accessing these data are described at the back of the journal.

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Acta Cryst. (1997). C**53**, 1299–1301

Isoalangidiol Monoacetate, a Triterpene Alcohol

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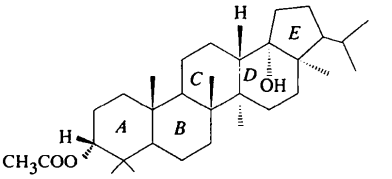
Abstract

Isoalangidiol (3α,18α-*B'*:*A'*-neogammacerane-3,18-diol) has been extracted as a natural product from the leaves of *Alangium lamarckii Thw.* (Alangiaceae). The crystal structure study of its monoacetate, $C_{32}H_{54}O_3$, was undertaken in order to ascertain the conformation of the compound. The four six-membered rings are in chair conformations. The five-membered ring is distorted from a plane and is twisted, with a C19—C18—C17—C21 torsion angle of −43.0 (4)°. The molecular parameters of the compound are all within normal limits.

Comment

Isoalangidiol has been obtained from the petroleum ether extract of *Alangium lamarckii Thw.* (Alangiaceae) and purified as its monoacetate, (I), prepared by heating with acetic anhydride/pyridine at 373 K, by column chromatography over silica gel (Pakrashi & Achari, 1971). The structural elucidation *via* NMR spectra has already been carried out (Achari, Pal & Pakrashi, 1975). The present X-ray structure study was carried out in order to confirm these findings. Isoalangidiol is the 3α-epimer of 18α-*B'*:*A'*-neogammacerane-3,18-diol. It represents the first example of a naturally occurring *D*:*E*-*cis* neohopane derivative and belongs to the rare group of pentacyclic triterpenes with a free hydroxyl group at the ring juncture.



(I)

The title compound consists of four *trans*-fused six-membered alicyclic rings (*A*, *B*, *C* and *D*) and a five-membered ring *E* *cis*-fused to ring *D*. Rings *A*, *B*, *C* and *D* are in chair conformations, as shown by the ring-puckering parameters given in Table 2 (Cremer & Pople, 1975). The acetoxy function, adjacent to a methylene group, is axial. There are altogether eight methyl groups in the structure. The isopropyl group is attached to ring *E*. The hydroxy group is attached to C18 in this neohopane derivative. The five-membered ring has a twisted conformation, with a C19—C18—C17—C21 torsion angle of −43.0 (4)°.

There is an intermolecular O—H···O hydrogen bond between the O18 and O32 atoms, joining the molecules into infinite chains along the *z* axis [O18···O32^{i} 2.961 (5) Å and O18—H18···O32^{i} 124.1 (4)°; symmetry code: (i) $-x-\frac{1}{2}, -y, z-\frac{1}{2}$].

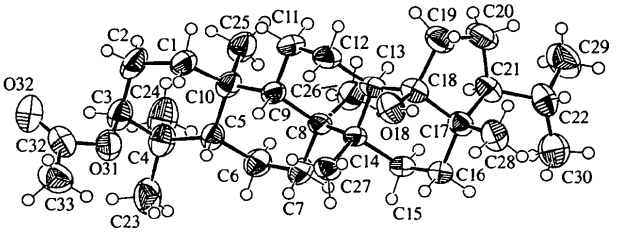


Fig. 1. The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

Isoalangidiol monoacetate, (I), was crystallized from a solution of benzene and ethanol.

Crystal data

$C_{32}H_{54}O_3$
M_r = 486.75
Mo $K\alpha$ radiation
λ = 0.71073 Å