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exo-8,*exo*-11-Diallylpentacyclo-[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane-*endo*-8,*endo*-11-diol

Grant A. Boyle,[a] Thavendran Govender,[b] Rajshekhar Karpoormath[a] and Hendrik G. Kruger[a]*

[a]School of Chemistry, University of KwaZulu-Natal, Durban 4000, South Africa, and [b]School of Pharmacy and Pharmacology, University of KwaZulu-Natal, Durban 4000, South Africa
Correspondence e-mail: kruger@ukzn.ac.za

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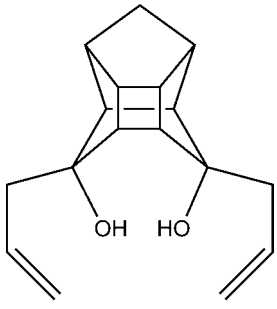
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.119; data-to-parameter ratio = 16.5.

The title compound, $C_{17}H_{22}O_2$, was synthesized as part of an ongoing investigation into the biological activity of cage compounds and their derivatives. The molecule exhibits C—C bond lengths that deviate from normal values. A number of long [*e.g.* 1.593 (2) Å] and short [*e.g.* 1.520 (3) Å] C—C bonds are observed. The molecule shows both inter- and intramolecular O—H···O hydrogen bonds involving all four molecules in the asymmetric unit.

Related literature

For related literature, see: Flippen-Anderson *et al.*, 1991; Linden *et al.*, 2005; Kruger *et al.*, 2005, 2006. Boyle *et al.*, 2007.



Experimental

Crystal data

$C_{17}H_{22}O_2$
M_r = 258.35
Monoclinic, $P2_1/n$
a = 14.3516 (9) Å
b = 21.8695 (16) Å
c = 18.4990 (13) Å
β = 91.024 (2)°
V = 5805.2 (7) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
0.46 × 0.44 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
53742 measured reflections
11417 independent reflections
8116 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 1.03
11417 reflections
693 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1A—H1AO···O2A	0.84	1.71	2.5163 (15)	160
O2A—H2AO···O1D	0.84	1.86	2.6727 (14)	161
O1B—H1BO···O1A	0.84	1.85	2.6198 (14)	151
O2B—H2BO···O1B	0.84	1.73	2.5356 (16)	160
O1C—H1CO···O2B	0.84	1.89	2.7297 (15)	175
O2C—H2CO···O1C	0.84	1.74	2.5446 (16)	161
O1D—H1DH···O2D	0.84	1.73	2.5318 (15)	160
O2D—H2DH···O2C	0.84	1.87	2.6984 (14)	170

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL* molecular graphics: *Mercury* (Macrae *et al.*, 2006) and *WinGX* (Farrugia, 1999); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2176).

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supplementary materials

Acta Cryst. (2007). E**63**, o4797 [**doi:10.1107/S1600536807055699**]

exo-8,*exo*-11-Diallylpentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane-*endo*-8,*endo*-11-diol

G. A. Boyle, T. Govender, R. Karpoormath and H. G. Kruger

Comment

The novel compound (**I**) was synthesized as a part of an ongoing project looking into the biological activity of cage compounds and their derivatives. It can be converted to a diacid and coupled to desired peptides as a potential HIV-1 protease inhibitor. The title compound (**I**) consists of a large apolar (lipophilic) hydrocarbon skeleton with polar dihydroxy units (Fig.1).

(I) crystallized with four molecules in the asymmetric unit (Fig. 2)all of which show shortening and elongation of specific C—C bonds in the cage moiety as observed by previous authors (Flippen-Anderson *et al.*, 1991; Linden *et al.*, 2005; Kruger *et al.*, 2005; Kruger *et al.*, 2006, Boyle *et al.*, 2007). The C—C bond lengths between C_1—$C_{11,}$ C_3—C_4, C_4—C_5 and C_7—C_8 are observed to be shortest with the values ranging between 1.516–1.531 Å and the C—C bond length between C_9—C_{10} is the longest with the values ranging between 1.591–1.597 Å. The propylene chains are in energetically favorable conformations thus allowing both inter- and intra-molecular hydrogen bonding between the hydroxyl groups of the four molecules of the asymmetric unit (Fig.2).

In three of the four molecules making up the asymmetric unit, C14 and C17 are on the same side of the plane formed by C12, C13, C15 and C16 while in the fourth molecule C14 and C17 are on opposite sides of the plane.

Interestingly it was observed that in *exo*-8-*exo*-11-vinylpentacyclo-[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]-undecane-*endo*-8-*endo*-11-diol (Boyle *et al.*, 2007 - Fig. 3), which contains a single molecule in the asymmetric unit, each molecule interacts with a neighbouring molecule by hydrogen bonding between the hydroxyl groups, forming a linear chain which in turn shows short interactions between the lipophilic parts of neighbouring molecules to form a bilayer. For **I**, the four independent molecules are held together by hydrogen bonding. The hydroxyl groups present in each molecule are both involved in hydrogen bonding. The intra- and intermolecular hydrogen bonding between the hydroxyl groups is only observed within the asymmetric unit, each hydroxyl group then acting as a hydrogen bond donor and acceptor. This is different from that seen in the vinyl derivative (Boyle *et al.*, 2007) in that there is no hydrogen bonding interactions between the asymmetric units. Each asymmetric unit interacts with other neighboring units *via* short lipophilic interactions, thus forming linear bilayer packing as shown in Fig. 4. There is no hydrogen bonding observed between the lipophilic parts of the bilayers.

Experimental

A solution of pentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane-8,11-dione (20.0 g, 0.115 mol) in dry THF (200 ml) was added dropwise over 2 h to a stirred suspension of freshly prepared allylmagnesium bromide under nitrogen at 0°C. After the addition had been completed, the external ice-water bath was removed, and the reaction mixture was allowed to warm gradually to ambient room temperature while stirring under nitrogen during 24 h. The reaction was quenched *via* addition of saturated aqueous NH_4Cl (until pH is 6~7), the layers were separated, and the aqueous layers was extracted with EtOAc (2 *x* 500 ml). The combined organic extracts were dried (Na_2SO_4) and filtered, and the filtrate was concentrated *in vacuo*. The residue was

recrystallized from hexane, thereby affording pure *exo*-8-*exo*-11- divinylpentacyclo [5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane-*endo*-8-*endo*-11-diol (27.0 g, 91%) as a colorless microcrystalline solid

Refinement

Hydrogen atoms were first located in a difference map then positioned geometrically and allowed to ride on their respective parent atoms, with C—H bond lengths of 1.00 (SP_3 CH), 0.95 (SP_2 CH), 0.99 (CH_2), or 0.84 (OH), and with U_{iso}(H) = 1.2 (CH and CH_2) or 1.5 (OH) times U_{eq}(C).

Figures

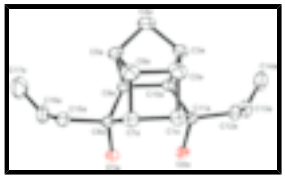


Fig. 1. : A representation of (I), showing the atomic numbering scheme and ellipsoids at the 50% probability level. H atoms have been removed.

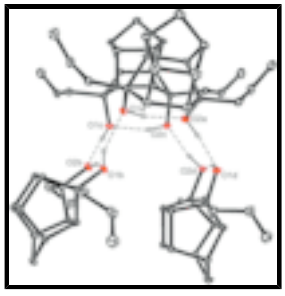


Fig. 2. : The asymmetric unit of (I), showing ellipsoids at the 30% probability level. Intermolecular and intramolecular hydrogen bonding is shown. H atoms have been removed for clarity.

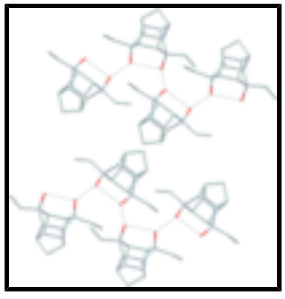


Fig. 3. :*exo*-8-*exo*-11-vinylpentacyclo-[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]-undecane-*endo*-8-*endo*-11-diol packing diagram.

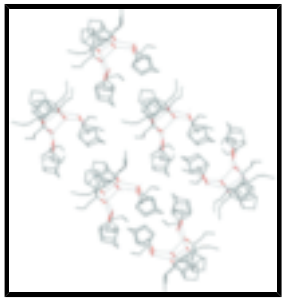


Fig. 4. : Depiction of packing showing intra- and intermolecular hydrogen bonding. Hydrogen atoms have been ommited for reasons of clarity.

exo-8,*exo*-11- Diallylpentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]undecane-*endo*- 8,*endo*-11-diol

Crystal data

$C_{17}H_{22}O_2$	F_{000} = 2240
M_r = 258.35	D_x = 1.182 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1020 reflections
a = 14.3516 (9) Å	θ = 2.2–27.7º
b = 21.8695 (16) Å	μ = 0.08 mm^{-1}
c = 18.4990 (13) Å	T = 173 (2) K
β = 91.024 (2)º	Block, colourless
V = 5805.2 (7) Å^3	0.46 × 0.44 × 0.30 mm
Z = 16	

Data collection

Bruker SMART CCD area-detector diffractometer	8116 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.042
Monochromator: graphite	θ_{max} = 26.0º
T = 173(2) K	θ_{min} = 1.7º
phi and ω scans	h = −17→17
Absorption correction: none	k = −26→26
53742 measured reflections	l = −22→22
11417 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H-atom parameters constrained
$wR(F^2)$ = 0.119	$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2 + 1.1142P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
11417 reflections	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
693 parameters	$\Delta\rho_{min}$ = −0.22 e Å^{-3}
7 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections(Bruker, 1999). The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1A	0.25857 (12)	0.05373 (7)	0.20312 (9)	0.0420 (4)
H1A	0.2033	0.0302	0.2200	0.050*
C2A	0.31333 (14)	0.02285 (8)	0.14167 (10)	0.0535 (5)
H2A	0.2879	−0.0163	0.1214	0.064*
C3A	0.34059 (13)	0.07341 (9)	0.08724 (9)	0.0501 (5)
H3A	0.3037	0.0739	0.0409	0.060*
C4A	0.44512 (14)	0.06562 (11)	0.07937 (10)	0.0657 (6)
H4A	0.4619	0.0261	0.0569	0.079*
H4B	0.4740	0.0999	0.0529	0.079*
C5A	0.46717 (13)	0.06727 (9)	0.15985 (9)	0.0526 (5)
H5A	0.5345	0.0627	0.1735	0.063*
C6A	0.40125 (14)	0.01878 (8)	0.19201 (10)	0.0551 (5)
H6A	0.4277	−0.0228	0.2016	0.066*
C7A	0.34694 (12)	0.04969 (7)	0.25408 (9)	0.0424 (4)
H7A	0.3392	0.0239	0.2982	0.051*
C8A	0.40031 (11)	0.10874 (7)	0.26620 (8)	0.0351 (3)
C9A	0.41959 (11)	0.12656 (8)	0.18731 (8)	0.0374 (4)
H9A	0.4608	0.1633	0.1837	0.045*
C10A	0.32944 (10)	0.13113 (7)	0.13577 (8)	0.0339 (3)
H10A	0.3273	0.1699	0.1072	0.041*
C11A	0.23627 (10)	0.11662 (7)	0.17202 (8)	0.0319 (3)
C12A	0.15349 (11)	0.11328 (8)	0.11796 (9)	0.0410 (4)
H12A	0.1657	0.0806	0.0823	0.049*
H12B	0.0967	0.1019	0.1444	0.049*
C13A	0.13569 (12)	0.17177 (9)	0.07846 (10)	0.0497 (4)
H13A	0.1202	0.2064	0.1069	0.060*
C14A	0.13929 (13)	0.17989 (11)	0.00922 (12)	0.0648 (6)
H14A	0.1545	0.1467	−0.0215	0.078*
H14B	0.1268	0.2191	−0.0109	0.078*
C15A	0.49009 (12)	0.09675 (9)	0.31095 (9)	0.0505 (5)
H15A	0.4729	0.0859	0.3609	0.061*
H15B	0.5229	0.0613	0.2901	0.061*
C16A	0.55496 (14)	0.14986 (12)	0.31359 (11)	0.0681 (6)

H16A	0.5304	0.1875	0.3304	0.082*
C17A	0.64198 (18)	0.1497 (2)	0.29507 (15)	0.1203 (12)
H17A	0.6697	0.1131	0.2779	0.144*
H17B	0.6778	0.1861	0.2987	0.144*
O1A	0.35432 (8)	0.15552 (5)	0.30626 (6)	0.0405 (3)
H1AO	0.3029	0.1637	0.2862	0.061*
O2A	0.21265 (7)	0.16239 (5)	0.22455 (6)	0.0373 (3)
H2AO	0.1551	0.1613	0.2319	0.056*
C1B	0.38981 (11)	0.23611 (9)	0.55991 (9)	0.0459 (4)
H1B	0.4510	0.2565	0.5513	0.055*
C2B	0.37293 (12)	0.21739 (9)	0.64037 (9)	0.0506 (5)
H2B	0.4214	0.2294	0.6771	0.061*
C3B	0.27001 (12)	0.23261 (9)	0.65731 (8)	0.0454 (4)
H3B	0.2605	0.2696	0.6880	0.054*
C4B	0.23213 (13)	0.17319 (9)	0.68769 (9)	0.0473 (4)
H4C	0.1636	0.1738	0.6927	0.057*
H4D	0.2625	0.1616	0.7342	0.057*
C5B	0.26329 (11)	0.13364 (8)	0.62493 (8)	0.0405 (4)
H5B	0.2481	0.0891	0.6287	0.049*
C6B	0.36840 (11)	0.14925 (9)	0.61815 (9)	0.0485 (4)
H6B	0.4142	0.1208	0.6418	0.058*
C7B	0.38541 (11)	0.16716 (8)	0.53770 (9)	0.0438 (4)
H7B	0.4439	0.1504	0.5167	0.053*
C8B	0.29515 (10)	0.14653 (8)	0.49981 (8)	0.0357 (4)
C9B	0.22428 (10)	0.16651 (7)	0.55653 (8)	0.0323 (3)
H9B	0.1594	0.1532	0.5437	0.039*
C10B	0.22899 (10)	0.23674 (7)	0.57923 (8)	0.0349 (3)
H10B	0.1664	0.2568	0.5775	0.042*
C11B	0.30421 (11)	0.27498 (8)	0.54116 (8)	0.0394 (4)
C12B	0.31634 (14)	0.33953 (9)	0.57364 (10)	0.0566 (5)
H12C	0.3426	0.3355	0.6233	0.068*
H12D	0.3622	0.3622	0.5446	0.068*
C13B	0.22825 (17)	0.37659 (10)	0.57679 (12)	0.0675 (6)
H13B	0.1819	0.3629	0.6091	0.081*
C14B	0.20979 (18)	0.42509 (12)	0.53987 (14)	0.0820 (7)
H14C	0.2540	0.4405	0.5069	0.098*
H14D	0.1519	0.4455	0.5456	0.098*
C15B	0.29607 (13)	0.07674 (8)	0.48741 (9)	0.0495 (4)
H15C	0.3405	0.0674	0.4486	0.059*
H15D	0.3193	0.0566	0.5321	0.059*
C16B	0.20345 (15)	0.04998 (9)	0.46724 (11)	0.0571 (5)
H16B	0.1727	0.0663	0.4256	0.069*
C17B	0.16096 (18)	0.00624 (11)	0.50152 (13)	0.0790 (7)
H17C	0.1891	−0.0115	0.5434	0.095*
H17D	0.1019	−0.0079	0.4846	0.095*
O1B	0.27492 (8)	0.17382 (5)	0.43084 (5)	0.0401 (3)
H1BO	0.3135	0.1614	0.4006	0.060*
O2B	0.28620 (8)	0.28570 (5)	0.46586 (6)	0.0436 (3)
H2BO	0.2816	0.2521	0.4441	0.065*

C1C	0.31199 (11)	0.30260 (7)	0.22762 (9)	0.0370 (4)
H1C	0.2809	0.2617	0.2254	0.044*
C2C	0.38762 (11)	0.31335 (7)	0.16926 (9)	0.0389 (4)
H2C	0.3967	0.2804	0.1326	0.047*
C3C	0.37583 (11)	0.37968 (7)	0.14083 (8)	0.0355 (4)
H3C	0.3467	0.3835	0.0915	0.043*
C4C	0.47297 (11)	0.40723 (8)	0.14939 (8)	0.0394 (4)
H4E	0.5192	0.3873	0.1181	0.047*
H4F	0.4735	0.4520	0.1417	0.047*
C5C	0.48512 (10)	0.38981 (7)	0.22847 (8)	0.0351 (3)
H5C	0.5458	0.4021	0.2515	0.042*
C6C	0.46367 (11)	0.32025 (7)	0.22991 (9)	0.0393 (4)
H6C	0.5178	0.2915	0.2290	0.047*
C7C	0.38868 (11)	0.30940 (7)	0.28879 (9)	0.0373 (4)
H7C	0.3987	0.2723	0.3196	0.045*
C8C	0.38856 (10)	0.37025 (7)	0.32953 (8)	0.0345 (3)
C9C	0.39680 (10)	0.41497 (7)	0.26564 (8)	0.0308 (3)
H9C	0.4046	0.4583	0.2819	0.037*
C10C	0.31923 (10)	0.40795 (7)	0.20322 (8)	0.0310 (3)
H10C	0.2898	0.4479	0.1896	0.037*
C11C	0.24658 (10)	0.35721 (7)	0.21652 (8)	0.0333 (3)
C12C	0.18180 (11)	0.34537 (8)	0.15082 (9)	0.0396 (4)
H12E	0.2200	0.3308	0.1102	0.047*
H12F	0.1381	0.3121	0.1632	0.047*
C13C	0.12672 (12)	0.39926 (9)	0.12588 (10)	0.0496 (4)
H13C	0.0935	0.4214	0.1613	0.060*
C14C	0.12049 (16)	0.41857 (11)	0.05896 (13)	0.0736 (6)
H14E	0.1527	0.3977	0.0220	0.088*
H14F	0.0837	0.4535	0.0474	0.088*
C15C	0.47316 (11)	0.37434 (8)	0.38234 (9)	0.0420 (4)
H15E	0.4635	0.3458	0.4230	0.050*
H15F	0.5298	0.3612	0.3569	0.050*
C16C	0.48845 (13)	0.43730 (9)	0.41183 (9)	0.0499 (4)
H16C	0.4377	0.4561	0.4355	0.060*
C17C	0.56609 (16)	0.46872 (11)	0.40773 (11)	0.0704 (6)
H17E	0.6185	0.4516	0.3845	0.084*
H17F	0.5699	0.5086	0.4280	0.084*
O1C	0.30795 (7)	0.38156 (5)	0.37316 (6)	0.0392 (3)
H1CO	0.3026	0.3534	0.4037	0.059*
O2C	0.18375 (7)	0.37009 (5)	0.27419 (6)	0.0399 (3)
H2CO	0.2144	0.3758	0.3127	0.060*
C1D	0.04372 (10)	0.25755 (7)	0.41026 (8)	0.0345 (3)
H1D	0.1039	0.2752	0.4288	0.041*
C2D	−0.03138 (11)	0.24616 (8)	0.46895 (8)	0.0391 (4)
H2D	−0.0160	0.2594	0.5195	0.047*
C3D	−0.12711 (10)	0.26616 (8)	0.43638 (8)	0.0358 (4)
H3D	−0.1519	0.3059	0.4547	0.043*
C4D	−0.18904 (11)	0.21091 (8)	0.44816 (9)	0.0415 (4)
H4G	−0.2499	0.2143	0.4224	0.050*

H4H	−0.1986	0.2021	0.5000	0.050*
C5D	−0.12407 (11)	0.16530 (8)	0.41293 (8)	0.0376 (4)
H5D	−0.1462	0.1220	0.4122	0.045*
C6D	−0.02900 (11)	0.17644 (8)	0.45253 (9)	0.0412 (4)
H6D	−0.0121	0.1484	0.4934	0.049*
C7D	0.04582 (10)	0.18720 (7)	0.39365 (8)	0.0367 (4)
H7D	0.1072	0.1668	0.4034	0.044*
C8D	−0.00460 (10)	0.16656 (7)	0.32429 (8)	0.0332 (3)
C9D	−0.10218 (10)	0.19328 (7)	0.33805 (8)	0.0297 (3)
H9D	−0.1489	0.1812	0.2999	0.036*
C10D	−0.10411 (9)	0.26464 (7)	0.35473 (7)	0.0283 (3)
H10D	−0.1518	0.2867	0.3245	0.034*
C11D	−0.00868 (10)	0.29691 (7)	0.35460 (7)	0.0298 (3)
C12D	−0.01476 (11)	0.36386 (7)	0.37991 (8)	0.0369 (4)
H12G	−0.0348	0.3646	0.4308	0.044*
H12H	0.0480	0.3825	0.3781	0.044*
C13D	−0.08085 (12)	0.40139 (7)	0.33520 (9)	0.0420 (4)
H13D	−0.0718	0.4020	0.2845	0.050*
C14D	−0.15018 (14)	0.43346 (9)	0.36021 (12)	0.0627 (5)
H14G	−0.1616	0.4340	0.4106	0.075*
H14H	−0.1891	0.4562	0.3279	0.075*
C15D	−0.00550 (12)	0.09609 (7)	0.31926 (9)	0.0427 (4)
H15G	0.0582	0.0817	0.3086	0.051*
H15H	−0.0228	0.0791	0.3668	0.051*
C16D	−0.07127 (13)	0.07206 (8)	0.26284 (11)	0.0504 (4)
H16D	−0.0644	0.0867	0.2149	0.061*
C17D	−0.13777 (15)	0.03229 (10)	0.27407 (13)	0.0674 (6)
H17G	−0.1469	0.0165	0.3212	0.081*
H17H	−0.1768	0.0193	0.2350	0.081*
O1D	0.03546 (7)	0.18537 (5)	0.25738 (6)	0.0374 (3)
H1DH	0.0397	0.2237	0.2565	0.056*
O2D	0.03088 (7)	0.29892 (5)	0.28374 (5)	0.0333 (2)
H2DH	0.0809	0.3189	0.2854	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1A	0.0475 (10)	0.0289 (9)	0.0495 (10)	−0.0050 (7)	0.0032 (8)	0.0010 (7)
C2A	0.0705 (13)	0.0340 (10)	0.0558 (11)	0.0065 (9)	−0.0035 (9)	−0.0140 (8)
C3A	0.0528 (11)	0.0629 (12)	0.0347 (9)	0.0122 (9)	0.0027 (8)	−0.0149 (8)
C4A	0.0618 (13)	0.0910 (16)	0.0447 (11)	0.0271 (11)	0.0098 (9)	−0.0147 (10)
C5A	0.0450 (10)	0.0741 (13)	0.0389 (10)	0.0250 (9)	0.0082 (8)	−0.0058 (9)
C6A	0.0684 (13)	0.0393 (10)	0.0576 (12)	0.0224 (9)	0.0002 (10)	−0.0064 (8)
C7A	0.0502 (10)	0.0342 (9)	0.0429 (9)	0.0074 (7)	0.0053 (8)	0.0068 (7)
C8A	0.0341 (8)	0.0389 (9)	0.0324 (8)	0.0095 (7)	0.0051 (6)	0.0003 (6)
C9A	0.0318 (8)	0.0463 (10)	0.0341 (8)	0.0013 (7)	0.0048 (6)	0.0022 (7)
C10A	0.0340 (8)	0.0378 (9)	0.0301 (8)	−0.0009 (6)	0.0033 (6)	0.0015 (6)
C11A	0.0326 (8)	0.0287 (8)	0.0345 (8)	−0.0011 (6)	0.0049 (6)	−0.0032 (6)

C12A	0.0360 (9)	0.0421 (10)	0.0449 (10)	−0.0072 (7)	−0.0003 (7)	−0.0036 (7)
C13A	0.0456 (10)	0.0496 (11)	0.0533 (11)	−0.0036 (8)	−0.0151 (8)	−0.0013 (8)
C14A	0.0463 (11)	0.0842 (16)	0.0633 (14)	−0.0129 (10)	−0.0129 (9)	0.0189 (11)
C15A	0.0426 (10)	0.0705 (13)	0.0384 (9)	0.0156 (9)	0.0019 (7)	0.0057 (9)
C16A	0.0391 (11)	0.1087 (19)	0.0562 (12)	−0.0049 (11)	−0.0109 (9)	0.0128 (12)
C17A	0.0537 (16)	0.227 (4)	0.0792 (19)	−0.026 (2)	−0.0081 (13)	0.012 (2)
O1A	0.0371 (6)	0.0484 (7)	0.0360 (6)	0.0068 (5)	0.0019 (5)	−0.0095 (5)
O2A	0.0319 (6)	0.0383 (6)	0.0419 (6)	0.0051 (5)	0.0052 (5)	−0.0073 (5)
C1B	0.0264 (8)	0.0744 (13)	0.0367 (9)	−0.0121 (8)	−0.0031 (7)	0.0049 (8)
C2B	0.0352 (9)	0.0844 (14)	0.0319 (9)	−0.0128 (9)	−0.0103 (7)	0.0031 (9)
C3B	0.0442 (10)	0.0635 (12)	0.0284 (8)	−0.0100 (8)	0.0006 (7)	−0.0078 (8)
C4B	0.0445 (10)	0.0703 (12)	0.0272 (8)	−0.0055 (9)	0.0011 (7)	0.0013 (8)
C5B	0.0366 (9)	0.0545 (11)	0.0304 (8)	0.0013 (7)	−0.0007 (7)	0.0048 (7)
C6B	0.0315 (9)	0.0766 (13)	0.0371 (9)	0.0068 (8)	−0.0069 (7)	0.0136 (9)
C7B	0.0263 (8)	0.0686 (12)	0.0365 (9)	0.0116 (8)	0.0013 (7)	0.0075 (8)
C8B	0.0324 (8)	0.0476 (10)	0.0271 (8)	0.0103 (7)	0.0014 (6)	0.0030 (7)
C9B	0.0245 (7)	0.0430 (9)	0.0295 (8)	0.0009 (6)	−0.0008 (6)	−0.0016 (6)
C10B	0.0282 (8)	0.0474 (10)	0.0292 (8)	−0.0005 (7)	0.0003 (6)	−0.0061 (7)
C11B	0.0371 (9)	0.0515 (10)	0.0297 (8)	−0.0082 (7)	−0.0012 (6)	−0.0026 (7)
C12B	0.0664 (13)	0.0575 (12)	0.0459 (11)	−0.0232 (10)	−0.0003 (9)	−0.0077 (9)
C13B	0.0830 (16)	0.0487 (12)	0.0714 (14)	−0.0128 (11)	0.0196 (12)	−0.0141 (10)
C14B	0.0846 (17)	0.0701 (16)	0.0918 (18)	−0.0071 (13)	0.0192 (14)	−0.0087 (13)
C15B	0.0551 (11)	0.0537 (11)	0.0397 (9)	0.0205 (9)	0.0055 (8)	0.0016 (8)
C16B	0.0738 (14)	0.0411 (11)	0.0560 (12)	0.0115 (10)	−0.0091 (10)	−0.0091 (9)
C17B	0.0952 (18)	0.0629 (15)	0.0789 (16)	−0.0129 (13)	0.0045 (13)	−0.0125 (12)
O1B	0.0411 (6)	0.0536 (7)	0.0256 (5)	0.0090 (5)	0.0014 (5)	−0.0004 (5)
O2B	0.0486 (7)	0.0493 (7)	0.0330 (6)	−0.0022 (6)	−0.0007 (5)	0.0022 (5)
C1C	0.0388 (9)	0.0298 (8)	0.0426 (9)	−0.0092 (7)	0.0085 (7)	−0.0043 (7)
C2C	0.0404 (9)	0.0331 (9)	0.0435 (9)	−0.0043 (7)	0.0110 (7)	−0.0114 (7)
C3C	0.0358 (8)	0.0369 (9)	0.0341 (8)	−0.0075 (7)	0.0090 (7)	−0.0053 (7)
C4C	0.0338 (9)	0.0429 (9)	0.0418 (9)	−0.0067 (7)	0.0117 (7)	−0.0032 (7)
C5C	0.0290 (8)	0.0357 (9)	0.0408 (9)	−0.0031 (6)	0.0071 (6)	−0.0022 (7)
C6C	0.0348 (9)	0.0336 (9)	0.0499 (10)	0.0018 (7)	0.0088 (7)	−0.0042 (7)
C7C	0.0380 (9)	0.0311 (8)	0.0431 (9)	−0.0028 (7)	0.0054 (7)	0.0030 (7)
C8C	0.0300 (8)	0.0369 (9)	0.0368 (8)	−0.0030 (6)	0.0062 (6)	−0.0005 (7)
C9C	0.0286 (8)	0.0293 (8)	0.0345 (8)	−0.0029 (6)	0.0036 (6)	−0.0035 (6)
C10C	0.0298 (8)	0.0300 (8)	0.0332 (8)	−0.0037 (6)	0.0042 (6)	−0.0040 (6)
C11C	0.0312 (8)	0.0357 (8)	0.0333 (8)	−0.0085 (6)	0.0083 (6)	−0.0053 (6)
C12C	0.0369 (9)	0.0441 (10)	0.0380 (9)	−0.0150 (7)	0.0074 (7)	−0.0077 (7)
C13C	0.0390 (10)	0.0538 (11)	0.0557 (11)	−0.0145 (8)	−0.0091 (8)	−0.0055 (9)
C14C	0.0665 (14)	0.0749 (15)	0.0788 (16)	−0.0224 (12)	−0.0188 (12)	0.0181 (12)
C15C	0.0385 (9)	0.0496 (10)	0.0379 (9)	−0.0025 (7)	0.0008 (7)	0.0037 (7)
C16C	0.0520 (11)	0.0593 (12)	0.0382 (10)	−0.0080 (9)	−0.0069 (8)	−0.0034 (8)
C17C	0.0778 (15)	0.0756 (15)	0.0574 (13)	−0.0296 (12)	−0.0084 (11)	−0.0037 (11)
O1C	0.0380 (6)	0.0465 (7)	0.0334 (6)	−0.0042 (5)	0.0096 (5)	0.0005 (5)
O2C	0.0313 (6)	0.0547 (7)	0.0339 (6)	−0.0067 (5)	0.0075 (4)	−0.0067 (5)
C1D	0.0253 (7)	0.0494 (10)	0.0286 (8)	−0.0036 (7)	−0.0039 (6)	0.0022 (7)
C2D	0.0378 (9)	0.0548 (10)	0.0247 (8)	−0.0031 (7)	0.0006 (6)	0.0042 (7)
C3D	0.0319 (8)	0.0438 (9)	0.0320 (8)	−0.0007 (7)	0.0080 (6)	0.0003 (7)

C4D	0.0361 (9)	0.0510 (10)	0.0380 (9)	−0.0029 (7)	0.0112 (7)	0.0063 (7)
C5D	0.0331 (8)	0.0399 (9)	0.0401 (9)	−0.0028 (7)	0.0048 (7)	0.0092 (7)
C6D	0.0389 (9)	0.0516 (10)	0.0329 (8)	0.0012 (7)	−0.0016 (7)	0.0143 (7)
C7D	0.0261 (8)	0.0475 (10)	0.0364 (8)	0.0056 (7)	−0.0027 (6)	0.0088 (7)
C8D	0.0267 (8)	0.0377 (9)	0.0351 (8)	0.0039 (6)	0.0021 (6)	0.0043 (6)
C9D	0.0223 (7)	0.0344 (8)	0.0325 (8)	−0.0007 (6)	−0.0009 (6)	0.0025 (6)
C10D	0.0222 (7)	0.0337 (8)	0.0289 (7)	0.0006 (6)	0.0010 (6)	0.0023 (6)
C11D	0.0247 (7)	0.0397 (9)	0.0250 (7)	−0.0039 (6)	0.0019 (6)	−0.0006 (6)
C12D	0.0356 (8)	0.0420 (9)	0.0332 (8)	−0.0097 (7)	0.0028 (7)	−0.0044 (7)
C13D	0.0475 (10)	0.0333 (9)	0.0451 (10)	−0.0076 (7)	0.0019 (8)	−0.0007 (7)
C14D	0.0665 (13)	0.0493 (12)	0.0724 (14)	0.0122 (10)	0.0050 (11)	−0.0003 (10)
C15D	0.0392 (9)	0.0383 (9)	0.0506 (10)	0.0091 (7)	0.0040 (8)	0.0033 (8)
C16D	0.0541 (11)	0.0391 (10)	0.0581 (11)	0.0048 (8)	0.0018 (9)	−0.0064 (8)
C17D	0.0648 (13)	0.0561 (13)	0.0812 (15)	−0.0085 (11)	0.0015 (11)	−0.0156 (11)
O1D	0.0332 (6)	0.0427 (6)	0.0365 (6)	0.0024 (5)	0.0079 (5)	−0.0003 (5)
O2D	0.0277 (5)	0.0444 (6)	0.0280 (5)	−0.0063 (4)	0.0049 (4)	0.0023 (4)

Geometric parameters (Å, °)

C1A—C11A	1.523 (2)	C1C—C11C	1.531 (2)
C1A—C2A	1.549 (2)	C1C—C2C	1.562 (2)
C1A—C7A	1.569 (2)	C1C—C7C	1.571 (2)
C1A—H1A	1.0000	C1C—H1C	1.0000
C2A—C3A	1.550 (3)	C2C—C3C	1.551 (2)
C2A—C6A	1.557 (3)	C2C—C6C	1.558 (2)
C2A—H2A	1.0000	C2C—H2C	1.0000
C3A—C4A	1.519 (3)	C3C—C4C	1.524 (2)
C3A—C10A	1.559 (2)	C3C—C10C	1.552 (2)
C3A—H3A	1.0000	C3C—H3C	1.0000
C4A—C5A	1.517 (3)	C4C—C5C	1.519 (2)
C4A—H4A	0.9900	C4C—H4E	0.9900
C4A—H4B	0.9900	C4C—H4F	0.9900
C5A—C6A	1.547 (3)	C5C—C6C	1.552 (2)
C5A—C9A	1.555 (2)	C5C—C9C	1.554 (2)
C5A—H5A	1.0000	C5C—H5C	1.0000
C6A—C7A	1.554 (2)	C6C—C7C	1.563 (2)
C6A—H6A	1.0000	C6C—H6C	1.0000
C7A—C8A	1.516 (2)	C7C—C8C	1.529 (2)
C7A—H7A	1.0000	C7C—H7C	1.0000
C8A—O1A	1.4314 (18)	C8C—O1C	1.4438 (17)
C8A—C9A	1.540 (2)	C8C—C9C	1.540 (2)
C8A—C15A	1.542 (2)	C8C—C15C	1.547 (2)
C9A—C10A	1.597 (2)	C9C—C10C	1.597 (2)
C9A—H9A	1.0000	C9C—H9C	1.0000
C10A—C11A	1.540 (2)	C10C—C11C	1.545 (2)
C10A—H10A	1.0000	C10C—H10C	1.0000
C11A—O2A	1.4398 (17)	C11C—O2C	1.4370 (17)
C11A—C12A	1.541 (2)	C11C—C12C	1.539 (2)
C12A—C13A	1.493 (2)	C12C—C13C	1.488 (3)

C12A—H12A	0.9900	C12C—H12E	0.9900
C12A—H12B	0.9900	C12C—H12F	0.9900
C13A—C14A	1.295 (3)	C13C—C14C	1.310 (3)
C13A—H13A	0.9500	C13C—H13C	0.9500
C14A—H14A	0.9500	C14C—H14E	0.9500
C14A—H14B	0.9500	C14C—H14F	0.9500
C15A—C16A	1.489 (3)	C15C—C16C	1.496 (2)
C15A—H15A	0.9900	C15C—H15E	0.9900
C15A—H15B	0.9900	C15C—H15F	0.9900
C16A—C17A	1.301 (3)	C16C—C17C	1.312 (3)
C16A—H16A	0.9500	C16C—H16C	0.9500
C17A—H17A	0.9500	C17C—H17E	0.9500
C17A—H17B	0.9500	C17C—H17F	0.9500
O1A—H1AO	0.8400	O1C—H1CO	0.8400
O2A—H2AO	0.8400	O2C—H2CO	0.8400
C1B—C11B	1.529 (2)	C1D—C11D	1.529 (2)
C1B—C7B	1.564 (3)	C1D—C2D	1.563 (2)
C1B—C2B	1.567 (2)	C1D—C7D	1.569 (2)
C1B—H1B	1.0000	C1D—H1D	1.0000
C2B—C6B	1.547 (3)	C2D—C3D	1.553 (2)
C2B—C3B	1.552 (2)	C2D—C6D	1.555 (2)
C2B—H2B	1.0000	C2D—H2D	1.0000
C3B—C4B	1.520 (3)	C3D—C4D	1.518 (2)
C3B—C10B	1.553 (2)	C3D—C10D	1.552 (2)
C3B—H3B	1.0000	C3D—H3D	1.0000
C4B—C5B	1.521 (2)	C4D—C5D	1.520 (2)
C4B—H4C	0.9900	C4D—H4G	0.9900
C4B—H4D	0.9900	C4D—H4H	0.9900
C5B—C9B	1.551 (2)	C5D—C9D	1.552 (2)
C5B—C6B	1.554 (2)	C5D—C6D	1.556 (2)
C5B—H5B	1.0000	C5D—H5D	1.0000
C6B—C7B	1.562 (2)	C6D—C7D	1.561 (2)
C6B—H6B	1.0000	C6D—H6D	1.0000
C7B—C8B	1.530 (2)	C7D—C8D	1.530 (2)
C7B—H7B	1.0000	C7D—H7D	1.0000
C8B—O1B	1.4336 (18)	C8D—O1D	1.4342 (18)
C8B—C9B	1.538 (2)	C8D—C9D	1.543 (2)
C8B—C15B	1.543 (2)	C8D—C15D	1.544 (2)
C9B—C10B	1.593 (2)	C9D—C10D	1.591 (2)
C9B—H9B	1.0000	C9D—H9D	1.0000
C10B—C11B	1.545 (2)	C10D—C11D	1.5408 (19)
C10B—H10B	1.0000	C10D—H10D	1.0000
C11B—O2B	1.4317 (19)	C11D—O2D	1.4385 (16)
C11B—C12B	1.543 (2)	C11D—C12D	1.540 (2)
C12B—C13B	1.504 (3)	C12D—C13D	1.493 (2)
C12B—H12C	0.9900	C12D—H12G	0.9900
C12B—H12D	0.9900	C12D—H12H	0.9900
C13B—C14B	1.287 (3)	C13D—C14D	1.309 (2)
C13B—H13B	0.9500	C13D—H13D	0.9500

C14B—H14C	0.9500	C14D—H14G	0.9500
C14B—H14D	0.9500	C14D—H14H	0.9500
C15B—C16B	1.494 (3)	C15D—C16D	1.491 (2)
C15B—H15C	0.9900	C15D—H15G	0.9900
C15B—H15D	0.9900	C15D—H15H	0.9900
C16B—C17B	1.305 (3)	C16D—C17D	1.310 (3)
C16B—H16B	0.9500	C16D—H16D	0.9500
C17B—H17C	0.9500	C17D—H17G	0.9500
C17B—H17D	0.9500	C17D—H17H	0.9500
O1B—H1BO	0.8400	O1D—H1DH	0.8400
O2B—H2BO	0.8400	O2D—H2DH	0.8400
C11A—C1A—C2A	102.86 (13)	C11C—C1C—C2C	102.82 (12)
C11A—C1A—C7A	116.11 (13)	C11C—C1C—C7C	116.28 (12)
C2A—C1A—C7A	90.06 (13)	C2C—C1C—C7C	89.84 (12)
C11A—C1A—H1A	114.9	C11C—C1C—H1C	114.9
C2A—C1A—H1A	114.9	C2C—C1C—H1C	114.9
C7A—C1A—H1A	114.9	C7C—C1C—H1C	114.9
C1A—C2A—C3A	107.64 (14)	C3C—C2C—C6C	102.96 (12)
C1A—C2A—C6A	90.13 (13)	C3C—C2C—C1C	107.58 (12)
C3A—C2A—C6A	102.59 (15)	C6C—C2C—C1C	90.19 (12)
C1A—C2A—H2A	117.5	C3C—C2C—H2C	117.4
C3A—C2A—H2A	117.5	C6C—C2C—H2C	117.4
C6A—C2A—H2A	117.5	C1C—C2C—H2C	117.4
C4A—C3A—C2A	104.08 (16)	C4C—C3C—C2C	103.91 (13)
C4A—C3A—C10A	104.94 (15)	C4C—C3C—C10C	104.79 (12)
C2A—C3A—C10A	100.01 (12)	C2C—C3C—C10C	100.12 (12)
C4A—C3A—H3A	115.3	C4C—C3C—H3C	115.4
C2A—C3A—H3A	115.3	C2C—C3C—H3C	115.4
C10A—C3A—H3A	115.3	C10C—C3C—H3C	115.4
C5A—C4A—C3A	95.29 (14)	C5C—C4C—C3C	95.16 (12)
C5A—C4A—H4A	112.7	C5C—C4C—H4E	112.7
C3A—C4A—H4A	112.7	C3C—C4C—H4E	112.7
C5A—C4A—H4B	112.7	C5C—C4C—H4F	112.7
C3A—C4A—H4B	112.7	C3C—C4C—H4F	112.7
H4A—C4A—H4B	110.2	H4E—C4C—H4F	110.2
C4A—C5A—C6A	104.06 (17)	C4C—C5C—C6C	104.06 (13)
C4A—C5A—C9A	104.80 (15)	C4C—C5C—C9C	104.89 (12)
C6A—C5A—C9A	99.84 (13)	C6C—C5C—C9C	100.12 (11)
C4A—C5A—H5A	115.4	C4C—C5C—H5C	115.3
C6A—C5A—H5A	115.4	C6C—C5C—H5C	115.3
C9A—C5A—H5A	115.4	C9C—C5C—H5C	115.3
C5A—C6A—C7A	107.72 (14)	C5C—C6C—C2C	102.66 (13)
C5A—C6A—C2A	103.02 (15)	C5C—C6C—C7C	107.46 (12)
C7A—C6A—C2A	90.30 (13)	C2C—C6C—C7C	90.28 (12)
C5A—C6A—H6A	117.3	C5C—C6C—H6C	117.5
C7A—C6A—H6A	117.3	C2C—C6C—H6C	117.5
C2A—C6A—H6A	117.3	C7C—C6C—H6C	117.5
C8A—C7A—C6A	102.77 (14)	C8C—C7C—C6C	102.60 (12)
C8A—C7A—C1A	116.20 (13)	C8C—C7C—C1C	115.48 (13)

C6A—C7A—C1A	89.50 (13)	C6C—C7C—C1C	89.69 (12)
C8A—C7A—H7A	115.0	C8C—C7C—H7C	115.2
C6A—C7A—H7A	115.0	C6C—C7C—H7C	115.2
C1A—C7A—H7A	115.0	C1C—C7C—H7C	115.2
O1A—C8A—C7A	116.67 (13)	O1C—C8C—C7C	115.62 (12)
O1A—C8A—C9A	113.71 (12)	O1C—C8C—C9C	113.18 (12)
C7A—C8A—C9A	100.04 (13)	C7C—C8C—C9C	100.00 (12)
O1A—C8A—C15A	103.43 (12)	O1C—C8C—C15C	105.35 (12)
C7A—C8A—C15A	110.47 (14)	C7C—C8C—C15C	110.71 (13)
C9A—C8A—C15A	112.90 (13)	C9C—C8C—C15C	112.19 (12)
C8A—C9A—C5A	100.71 (13)	C8C—C9C—C5C	100.91 (12)
C8A—C9A—C10A	115.10 (12)	C8C—C9C—C10C	115.58 (12)
C5A—C9A—C10A	102.29 (13)	C5C—C9C—C10C	102.10 (11)
C8A—C9A—H9A	112.6	C8C—C9C—H9C	112.4
C5A—C9A—H9A	112.6	C5C—C9C—H9C	112.4
C10A—C9A—H9A	112.6	C10C—C9C—H9C	112.4
C11A—C10A—C3A	100.54 (12)	C11C—C10C—C3C	101.31 (11)
C11A—C10A—C9A	115.33 (12)	C11C—C10C—C9C	114.67 (12)
C3A—C10A—C9A	101.70 (12)	C3C—C10C—C9C	102.05 (11)
C11A—C10A—H10A	112.7	C11C—C10C—H10C	112.6
C3A—C10A—H10A	112.7	C3C—C10C—H10C	112.6
C9A—C10A—H10A	112.7	C9C—C10C—H10C	112.6
O2A—C11A—C1A	115.05 (12)	O2C—C11C—C1C	116.41 (12)
O2A—C11A—C10A	111.56 (12)	O2C—C11C—C12C	103.95 (12)
C1A—C11A—C10A	99.93 (12)	C1C—C11C—C12C	109.58 (12)
O2A—C11A—C12A	106.43 (12)	O2C—C11C—C10C	114.31 (12)
C1A—C11A—C12A	110.91 (12)	C1C—C11C—C10C	99.65 (12)
C10A—C11A—C12A	113.12 (12)	C12C—C11C—C10C	113.26 (12)
C13A—C12A—C11A	113.59 (13)	C13C—C12C—C11C	114.94 (13)
C13A—C12A—H12A	108.8	C13C—C12C—H12E	108.5
C11A—C12A—H12A	108.8	C11C—C12C—H12E	108.5
C13A—C12A—H12B	108.8	C13C—C12C—H12F	108.5
C11A—C12A—H12B	108.8	C11C—C12C—H12F	108.5
H12A—C12A—H12B	107.7	H12E—C12C—H12F	107.5
C14A—C13A—C12A	126.30 (19)	C14C—C13C—C12C	125.1 (2)
C14A—C13A—H13A	116.8	C14C—C13C—H13C	117.4
C12A—C13A—H13A	116.8	C12C—C13C—H13C	117.4
C13A—C14A—H14A	120.0	C13C—C14C—H14E	120.0
C13A—C14A—H14B	120.0	C13C—C14C—H14F	120.0
H14A—C14A—H14B	120.0	H14E—C14C—H14F	120.0
C16A—C15A—C8A	113.66 (16)	C16C—C15C—C8C	113.07 (14)
C16A—C15A—H15A	108.8	C16C—C15C—H15E	109.0
C8A—C15A—H15A	108.8	C8C—C15C—H15E	109.0
C16A—C15A—H15B	108.8	C16C—C15C—H15F	109.0
C8A—C15A—H15B	108.8	C8C—C15C—H15F	109.0
H15A—C15A—H15B	107.7	H15E—C15C—H15F	107.8
C17A—C16A—C15A	126.3 (3)	C17C—C16C—C15C	125.5 (2)
C17A—C16A—H16A	116.9	C17C—C16C—H16C	117.3
C15A—C16A—H16A	116.9	C15C—C16C—H16C	117.3

C16A—C17A—H17A	120.0	C16C—C17C—H17E	120.0
C16A—C17A—H17B	120.0	C16C—C17C—H17F	120.0
H17A—C17A—H17B	120.0	H17E—C17C—H17F	120.0
C8A—O1A—H1AO	109.5	C8C—O1C—H1CO	109.5
C11A—O2A—H2AO	109.5	C11C—O2C—H2CO	109.5
C11B—C1B—C7B	116.61 (13)	C11D—C1D—C2D	102.74 (12)
C11B—C1B—C2B	102.92 (13)	C11D—C1D—C7D	115.53 (12)
C7B—C1B—C2B	89.51 (14)	C2D—C1D—C7D	89.75 (12)
C11B—C1B—H1B	114.8	C11D—C1D—H1D	115.1
C7B—C1B—H1B	114.8	C2D—C1D—H1D	115.1
C2B—C1B—H1B	114.8	C7D—C1D—H1D	115.1
C6B—C2B—C3B	102.99 (14)	C3D—C2D—C6D	102.87 (13)
C6B—C2B—C1B	90.33 (13)	C3D—C2D—C1D	107.55 (12)
C3B—C2B—C1B	107.45 (13)	C6D—C2D—C1D	90.16 (12)
C6B—C2B—H2B	117.4	C3D—C2D—H2D	117.4
C3B—C2B—H2B	117.4	C6D—C2D—H2D	117.4
C1B—C2B—H2B	117.4	C1D—C2D—H2D	117.4
C4B—C3B—C2B	103.84 (15)	C4D—C3D—C10D	104.94 (12)
C4B—C3B—C10B	105.16 (13)	C4D—C3D—C2D	103.66 (13)
C2B—C3B—C10B	99.85 (12)	C10D—C3D—C2D	99.76 (11)
C4B—C3B—H3B	115.4	C4D—C3D—H3D	115.5
C2B—C3B—H3B	115.4	C10D—C3D—H3D	115.5
C10B—C3B—H3B	115.4	C2D—C3D—H3D	115.5
C3B—C4B—C5B	95.27 (13)	C3D—C4D—C5D	95.48 (12)
C3B—C4B—H4C	112.7	C3D—C4D—H4G	112.6
C5B—C4B—H4C	112.7	C5D—C4D—H4G	112.6
C3B—C4B—H4D	112.7	C3D—C4D—H4H	112.6
C5B—C4B—H4D	112.7	C5D—C4D—H4H	112.6
H4C—C4B—H4D	110.2	H4G—C4D—H4H	110.1
C4B—C5B—C9B	104.62 (13)	C4D—C5D—C9D	105.04 (12)
C4B—C5B—C6B	103.63 (14)	C4D—C5D—C6D	103.58 (13)
C9B—C5B—C6B	99.73 (12)	C9D—C5D—C6D	99.71 (11)
C4B—C5B—H5B	115.6	C4D—C5D—H5D	115.5
C9B—C5B—H5B	115.6	C9D—C5D—H5D	115.5
C6B—C5B—H5B	115.6	C6D—C5D—H5D	115.5
C2B—C6B—C5B	103.09 (14)	C2D—C6D—C5D	102.90 (13)
C2B—C6B—C7B	90.29 (14)	C2D—C6D—C7D	90.35 (12)
C5B—C6B—C7B	107.49 (12)	C5D—C6D—C7D	107.66 (12)
C2B—C6B—H6B	117.4	C2D—C6D—H6D	117.3
C5B—C6B—H6B	117.4	C5D—C6D—H6D	117.3
C7B—C6B—H6B	117.4	C7D—C6D—H6D	117.3
C8B—C7B—C6B	102.54 (13)	C8D—C7D—C6D	102.69 (12)
C8B—C7B—C1B	115.77 (13)	C8D—C7D—C1D	116.29 (12)
C6B—C7B—C1B	89.87 (13)	C6D—C7D—C1D	89.73 (12)
C8B—C7B—H7B	115.1	C8D—C7D—H7D	114.9
C6B—C7B—H7B	115.1	C6D—C7D—H7D	114.9
C1B—C7B—H7B	115.1	C1D—C7D—H7D	114.9
O1B—C8B—C7B	116.19 (13)	O1D—C8D—C7D	116.63 (12)
O1B—C8B—C9B	111.29 (12)	O1D—C8D—C9D	114.38 (12)

C7B—C8B—C9B	99.69 (12)	C7D—C8D—C9D	99.61 (12)
O1B—C8B—C15B	106.35 (12)	O1D—C8D—C15D	103.73 (12)
C7B—C8B—C15B	110.51 (13)	C7D—C8D—C15D	110.38 (12)
C9B—C8B—C15B	112.95 (13)	C9D—C8D—C15D	112.42 (12)
C8B—C9B—C5B	101.04 (12)	C8D—C9D—C5D	101.35 (11)
C8B—C9B—C10B	115.36 (12)	C8D—C9D—C10D	115.00 (11)
C5B—C9B—C10B	102.64 (12)	C5D—C9D—C10D	102.07 (11)
C8B—C9B—H9B	112.3	C8D—C9D—H9D	112.5
C5B—C9B—H9B	112.3	C5D—C9D—H9D	112.5
C10B—C9B—H9B	112.3	C10D—C9D—H9D	112.5
C11B—C10B—C3B	101.48 (12)	C11D—C10D—C3D	101.31 (11)
C11B—C10B—C9B	115.36 (12)	C11D—C10D—C9D	115.49 (11)
C3B—C10B—C9B	101.70 (13)	C3D—C10D—C9D	102.39 (11)
C11B—C10B—H10B	112.4	C11D—C10D—H10D	112.2
C3B—C10B—H10B	112.4	C3D—C10D—H10D	112.2
C9B—C10B—H10B	112.4	C9D—C10D—H10D	112.2
O2B—C11B—C1B	116.25 (13)	O2D—C11D—C1D	115.68 (12)
O2B—C11B—C12B	104.25 (14)	O2D—C11D—C12D	105.87 (11)
C1B—C11B—C12B	109.61 (14)	C1D—C11D—C12D	111.12 (12)
O2B—C11B—C10B	114.63 (12)	O2D—C11D—C10D	112.37 (11)
C1B—C11B—C10B	99.26 (13)	C1D—C11D—C10D	99.64 (11)
C12B—C11B—C10B	113.12 (13)	C12D—C11D—C10D	112.32 (12)
C13B—C12B—C11B	114.78 (15)	C13D—C12D—C11D	113.14 (13)
C13B—C12B—H12C	108.6	C13D—C12D—H12G	109.0
C11B—C12B—H12C	108.6	C11D—C12D—H12G	109.0
C13B—C12B—H12D	108.6	C13D—C12D—H12H	109.0
C11B—C12B—H12D	108.6	C11D—C12D—H12H	109.0
H12C—C12B—H12D	107.5	H12G—C12D—H12H	107.8
C14B—C13B—C12B	126.1 (2)	C14D—C13D—C12D	125.33 (17)
C14B—C13B—H13B	117.0	C14D—C13D—H13D	117.3
C12B—C13B—H13B	117.0	C12D—C13D—H13D	117.3
C13B—C14B—H14C	120.0	C13D—C14D—H14G	120.0
C13B—C14B—H14D	120.0	C13D—C14D—H14H	120.0
H14C—C14B—H14D	120.0	H14G—C14D—H14H	120.0
C16B—C15B—C8B	114.50 (14)	C16D—C15D—C8D	113.49 (14)
C16B—C15B—H15C	108.6	C16D—C15D—H15G	108.9
C8B—C15B—H15C	108.6	C8D—C15D—H15G	108.9
C16B—C15B—H15D	108.6	C16D—C15D—H15H	108.9
C8B—C15B—H15D	108.6	C8D—C15D—H15H	108.9
H15C—C15B—H15D	107.6	H15G—C15D—H15H	107.7
C17B—C16B—C15B	126.0 (2)	C17D—C16D—C15D	125.23 (19)
C17B—C16B—H16B	117.0	C17D—C16D—H16D	117.4
C15B—C16B—H16B	117.0	C15D—C16D—H16D	117.4
C16B—C17B—H17C	120.0	C16D—C17D—H17G	120.0
C16B—C17B—H17D	120.0	C16D—C17D—H17H	120.0
H17C—C17B—H17D	120.0	H17G—C17D—H17H	120.0
C8B—O1B—H1BO	109.5	C8D—O1D—H1DH	109.5
C11B—O2B—H2BO	109.5	C11D—O2D—H2DH	109.5
C11A—C1A—C2A—C3A	13.54 (18)	C11C—C1C—C2C—C3C	13.17 (16)

C7A—C1A—C2A—C3A	−103.31 (15)	C7C—C1C—C2C—C3C	−103.80 (13)
C11A—C1A—C2A—C6A	116.80 (14)	C11C—C1C—C2C—C6C	116.84 (12)
C7A—C1A—C2A—C6A	−0.05 (13)	C7C—C1C—C2C—C6C	−0.13 (11)
C1A—C2A—C3A—C4A	127.33 (15)	C6C—C2C—C3C—C4C	32.89 (14)
C6A—C2A—C3A—C4A	33.11 (17)	C1C—C2C—C3C—C4C	127.28 (13)
C1A—C2A—C3A—C10A	19.02 (17)	C6C—C2C—C3C—C10C	−75.25 (13)
C6A—C2A—C3A—C10A	−75.19 (15)	C1C—C2C—C3C—C10C	19.14 (15)
C2A—C3A—C4A—C5A	−52.18 (18)	C2C—C3C—C4C—C5C	−52.18 (13)
C10A—C3A—C4A—C5A	52.44 (18)	C10C—C3C—C4C—C5C	52.45 (14)
C3A—C4A—C5A—C6A	52.05 (18)	C3C—C4C—C5C—C6C	52.46 (14)
C3A—C4A—C5A—C9A	−52.32 (19)	C3C—C4C—C5C—C9C	−52.26 (14)
C4A—C5A—C6A—C7A	−127.54 (15)	C4C—C5C—C6C—C2C	−33.50 (14)
C9A—C5A—C6A—C7A	−19.44 (17)	C9C—C5C—C6C—C2C	74.79 (13)
C4A—C5A—C6A—C2A	−32.98 (17)	C4C—C5C—C6C—C7C	−127.85 (13)
C9A—C5A—C6A—C2A	75.12 (15)	C9C—C5C—C6C—C7C	−19.56 (16)
C1A—C2A—C6A—C5A	−108.23 (14)	C3C—C2C—C6C—C5C	0.25 (14)
C3A—C2A—C6A—C5A	−0.11 (16)	C1C—C2C—C6C—C5C	−107.85 (12)
C1A—C2A—C6A—C7A	0.05 (13)	C3C—C2C—C6C—C7C	108.23 (12)
C3A—C2A—C6A—C7A	108.16 (14)	C1C—C2C—C6C—C7C	0.13 (11)
C5A—C6A—C7A—C8A	−13.06 (18)	C5C—C6C—C7C—C8C	−12.84 (16)
C2A—C6A—C7A—C8A	−116.84 (14)	C2C—C6C—C7C—C8C	−116.21 (12)
C5A—C6A—C7A—C1A	103.74 (15)	C5C—C6C—C7C—C1C	103.24 (13)
C2A—C6A—C7A—C1A	−0.05 (13)	C2C—C6C—C7C—C1C	−0.13 (11)
C11A—C1A—C7A—C8A	−0.3 (2)	C11C—C1C—C7C—C8C	−0.29 (18)
C2A—C1A—C7A—C8A	104.05 (15)	C2C—C1C—C7C—C8C	103.96 (14)
C11A—C1A—C7A—C6A	−104.33 (15)	C11C—C1C—C7C—C6C	−104.12 (13)
C2A—C1A—C7A—C6A	0.05 (13)	C2C—C1C—C7C—C6C	0.13 (11)
C6A—C7A—C8A—O1A	163.65 (13)	C6C—C7C—C8C—O1C	162.21 (13)
C1A—C7A—C8A—O1A	67.82 (18)	C1C—C7C—C8C—O1C	66.45 (17)
C6A—C7A—C8A—C9A	40.57 (15)	C6C—C7C—C8C—C9C	40.36 (14)
C1A—C7A—C8A—C9A	−55.26 (16)	C1C—C7C—C8C—C9C	−55.40 (15)
C6A—C7A—C8A—C15A	−78.64 (15)	C6C—C7C—C8C—C15C	−78.10 (15)
C1A—C7A—C8A—C15A	−174.47 (13)	C1C—C7C—C8C—C15C	−173.87 (12)
O1A—C8A—C9A—C5A	−179.24 (13)	O1C—C8C—C9C—C5C	−177.67 (12)
C7A—C8A—C9A—C5A	−54.09 (15)	C7C—C8C—C9C—C5C	−54.09 (13)
C15A—C8A—C9A—C5A	63.32 (17)	C15C—C8C—C9C—C5C	63.29 (15)
O1A—C8A—C9A—C10A	−70.10 (17)	O1C—C8C—C9C—C10C	−68.46 (16)
C7A—C8A—C9A—C10A	55.05 (16)	C7C—C8C—C9C—C10C	55.12 (15)
C15A—C8A—C9A—C10A	172.46 (14)	C15C—C8C—C9C—C10C	172.49 (12)
C4A—C5A—C9A—C8A	151.96 (15)	C4C—C5C—C9C—C8C	152.37 (12)
C6A—C5A—C9A—C8A	44.46 (15)	C6C—C5C—C9C—C8C	44.74 (14)
C4A—C5A—C9A—C10A	33.08 (18)	C4C—C5C—C9C—C10C	32.96 (14)
C6A—C5A—C9A—C10A	−74.43 (14)	C6C—C5C—C9C—C10C	−74.67 (13)
C4A—C3A—C10A—C11A	−151.93 (15)	C4C—C3C—C10C—C11C	−151.81 (13)
C2A—C3A—C10A—C11A	−44.31 (15)	C2C—C3C—C10C—C11C	−44.37 (14)
C4A—C3A—C10A—C9A	−33.05 (17)	C4C—C3C—C10C—C9C	−33.25 (15)
C2A—C3A—C10A—C9A	74.57 (14)	C2C—C3C—C10C—C9C	74.18 (13)
C8A—C9A—C10A—C11A	−0.44 (19)	C8C—C9C—C10C—C11C	0.34 (17)
C5A—C9A—C10A—C11A	107.75 (14)	C5C—C9C—C10C—C11C	108.84 (13)

C8A—C9A—C10A—C3A	−108.18 (15)	C8C—C9C—C10C—C3C	−108.24 (13)
C5A—C9A—C10A—C3A	0.01 (15)	C5C—C9C—C10C—C3C	0.26 (14)
C2A—C1A—C11A—O2A	−160.61 (13)	C2C—C1C—C11C—O2C	−163.60 (12)
C7A—C1A—C11A—O2A	−64.12 (18)	C7C—C1C—C11C—O2C	−67.33 (16)
C2A—C1A—C11A—C10A	−41.04 (15)	C2C—C1C—C11C—C12C	78.87 (14)
C7A—C1A—C11A—C10A	55.46 (16)	C7C—C1C—C11C—C12C	175.13 (12)
C2A—C1A—C11A—C12A	78.54 (16)	C2C—C1C—C11C—C10C	−40.19 (14)
C7A—C1A—C11A—C12A	175.03 (13)	C7C—C1C—C11C—C10C	56.07 (15)
C3A—C10A—C11A—O2A	176.16 (12)	C3C—C10C—C11C—O2C	178.61 (13)
C9A—C10A—C11A—O2A	67.71 (16)	C9C—C10C—C11C—O2C	69.58 (16)
C3A—C10A—C11A—C1A	54.07 (14)	C3C—C10C—C11C—C1C	53.73 (14)
C9A—C10A—C11A—C1A	−54.38 (15)	C9C—C10C—C11C—C1C	−55.30 (14)
C3A—C10A—C11A—C12A	−63.88 (15)	C3C—C10C—C11C—C12C	−62.57 (16)
C9A—C10A—C11A—C12A	−172.32 (13)	C9C—C10C—C11C—C12C	−171.60 (12)
O2A—C11A—C12A—C13A	61.54 (17)	O2C—C11C—C12C—C13C	65.59 (16)
C1A—C11A—C12A—C13A	−172.65 (15)	C1C—C11C—C12C—C13C	−169.33 (13)
C10A—C11A—C12A—C13A	−61.32 (18)	C10C—C11C—C12C—C13C	−59.05 (18)
C11A—C12A—C13A—C14A	118.69 (19)	C11C—C12C—C13C—C14C	130.31 (18)
O1A—C8A—C15A—C16A	−65.19 (18)	O1C—C8C—C15C—C16C	−66.67 (16)
C7A—C8A—C15A—C16A	169.24 (15)	C7C—C8C—C15C—C16C	167.66 (14)
C9A—C8A—C15A—C16A	58.2 (2)	C9C—C8C—C15C—C16C	56.88 (18)
C8A—C15A—C16A—C17A	−124.6 (2)	C8C—C15C—C16C—C17C	−124.4 (2)
C11B—C1B—C2B—C6B	117.11 (14)	C11D—C1D—C2D—C3D	12.73 (16)
C7B—C1B—C2B—C6B	−0.12 (12)	C7D—C1D—C2D—C3D	−103.44 (13)
C11B—C1B—C2B—C3B	13.38 (18)	C11D—C1D—C2D—C6D	116.29 (12)
C7B—C1B—C2B—C3B	−103.85 (15)	C7D—C1D—C2D—C6D	0.13 (11)
C6B—C2B—C3B—C4B	33.09 (15)	C6D—C2D—C3D—C4D	33.49 (14)
C1B—C2B—C3B—C4B	127.61 (15)	C1D—C2D—C3D—C4D	127.81 (13)
C6B—C2B—C3B—C10B	−75.33 (15)	C6D—C2D—C3D—C10D	−74.63 (13)
C1B—C2B—C3B—C10B	19.18 (18)	C1D—C2D—C3D—C10D	19.69 (15)
C2B—C3B—C4B—C5B	−52.24 (14)	C10D—C3D—C4D—C5D	51.51 (14)
C10B—C3B—C4B—C5B	52.19 (15)	C2D—C3D—C4D—C5D	−52.70 (14)
C3B—C4B—C5B—C9B	−51.89 (15)	C3D—C4D—C5D—C9D	−51.74 (14)
C3B—C4B—C5B—C6B	52.18 (15)	C3D—C4D—C5D—C6D	52.42 (14)
C3B—C2B—C6B—C5B	0.08 (15)	C3D—C2D—C6D—C5D	−0.29 (14)
C1B—C2B—C6B—C5B	−107.92 (13)	C1D—C2D—C6D—C5D	−108.35 (12)
C3B—C2B—C6B—C7B	108.12 (13)	C3D—C2D—C6D—C7D	107.93 (12)
C1B—C2B—C6B—C7B	0.12 (12)	C1D—C2D—C6D—C7D	−0.13 (11)
C4B—C5B—C6B—C2B	−33.18 (16)	C4D—C5D—C6D—C2D	−32.93 (14)
C9B—C5B—C6B—C2B	74.59 (14)	C9D—C5D—C6D—C2D	75.26 (13)
C4B—C5B—C6B—C7B	−127.69 (15)	C4D—C5D—C6D—C7D	−127.49 (13)
C9B—C5B—C6B—C7B	−19.92 (18)	C9D—C5D—C6D—C7D	−19.30 (16)
C2B—C6B—C7B—C8B	−116.53 (13)	C2D—C6D—C7D—C8D	−116.81 (12)
C5B—C6B—C7B—C8B	−12.71 (18)	C5D—C6D—C7D—C8D	−13.14 (16)
C2B—C6B—C7B—C1B	−0.12 (12)	C2D—C6D—C7D—C1D	0.13 (11)
C5B—C6B—C7B—C1B	103.71 (15)	C5D—C6D—C7D—C1D	103.79 (13)
C11B—C1B—C7B—C8B	−0.2 (2)	C11D—C1D—C7D—C8D	−0.10 (18)
C2B—C1B—C7B—C8B	104.00 (14)	C2D—C1D—C7D—C8D	103.92 (13)
C11B—C1B—C7B—C6B	−104.11 (14)	C11D—C1D—C7D—C6D	−104.15 (13)

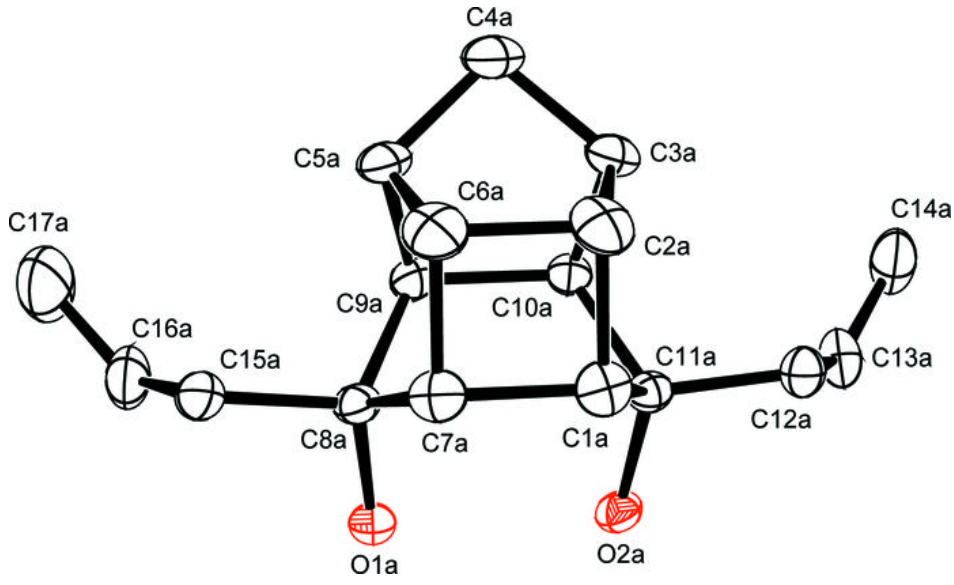
C2B—C1B—C7B—C6B	0.12 (12)	C2D—C1D—C7D—C6D	−0.13 (11)
C6B—C7B—C8B—O1B	160.13 (13)	C6D—C7D—C8D—O1D	164.00 (12)
C1B—C7B—C8B—O1B	64.11 (17)	C1D—C7D—C8D—O1D	67.92 (17)
C6B—C7B—C8B—C9B	40.49 (16)	C6D—C7D—C8D—C9D	40.40 (14)
C1B—C7B—C8B—C9B	−55.53 (16)	C1D—C7D—C8D—C9D	−55.68 (15)
C6B—C7B—C8B—C15B	−78.61 (16)	C6D—C7D—C8D—C15D	−78.00 (15)
C1B—C7B—C8B—C15B	−174.63 (13)	C1D—C7D—C8D—C15D	−174.08 (12)
O1B—C8B—C9B—C5B	−177.83 (13)	O1D—C8D—C9D—C5D	−179.40 (12)
C7B—C8B—C9B—C5B	−54.66 (15)	C7D—C8D—C9D—C5D	−54.24 (14)
C15B—C8B—C9B—C5B	62.62 (16)	C15D—C8D—C9D—C5D	62.64 (15)
O1B—C8B—C9B—C10B	−68.00 (16)	O1D—C8D—C9D—C10D	−70.20 (16)
C7B—C8B—C9B—C10B	55.17 (15)	C7D—C8D—C9D—C10D	54.97 (15)
C15B—C8B—C9B—C10B	172.44 (13)	C15D—C8D—C9D—C10D	171.84 (12)
C4B—C5B—C9B—C8B	152.32 (13)	C4D—C5D—C9D—C8D	151.71 (12)
C6B—C5B—C9B—C8B	45.35 (15)	C6D—C5D—C9D—C8D	44.69 (14)
C4B—C5B—C9B—C10B	32.92 (15)	C4D—C5D—C9D—C10D	32.79 (14)
C6B—C5B—C9B—C10B	−74.05 (14)	C6D—C5D—C9D—C10D	−74.24 (13)
C4B—C3B—C10B—C11B	−152.16 (14)	C4D—C3D—C10D—C11D	−152.06 (12)
C2B—C3B—C10B—C11B	−44.78 (16)	C2D—C3D—C10D—C11D	−44.97 (14)
C4B—C3B—C10B—C9B	−32.92 (16)	C4D—C3D—C10D—C9D	−32.51 (14)
C2B—C3B—C10B—C9B	74.45 (14)	C2D—C3D—C10D—C9D	74.59 (13)
C8B—C9B—C10B—C11B	−0.09 (18)	C8D—C9D—C10D—C11D	0.15 (17)
C5B—C9B—C10B—C11B	108.79 (14)	C5D—C9D—C10D—C11D	108.92 (13)
C8B—C9B—C10B—C3B	−108.94 (14)	C8D—C9D—C10D—C3D	−108.95 (13)
C5B—C9B—C10B—C3B	−0.06 (14)	C5D—C9D—C10D—C3D	−0.18 (13)
C7B—C1B—C11B—O2B	−67.91 (18)	C2D—C1D—C11D—O2D	−160.85 (12)
C2B—C1B—C11B—O2B	−163.94 (14)	C7D—C1D—C11D—O2D	−64.93 (16)
C7B—C1B—C11B—C12B	174.24 (14)	C2D—C1D—C11D—C12D	78.43 (14)
C2B—C1B—C11B—C12B	78.21 (16)	C7D—C1D—C11D—C12D	174.34 (12)
C7B—C1B—C11B—C10B	55.53 (16)	C2D—C1D—C11D—C10D	−40.17 (14)
C2B—C1B—C11B—C10B	−40.50 (15)	C7D—C1D—C11D—C10D	55.74 (15)
C3B—C10B—C11B—O2B	178.83 (13)	C3D—C10D—C11D—O2D	177.26 (12)
C9B—C10B—C11B—O2B	69.85 (17)	C9D—C10D—C11D—O2D	67.52 (15)
C3B—C10B—C11B—C1B	54.24 (15)	C3D—C10D—C11D—C1D	54.21 (13)
C9B—C10B—C11B—C1B	−54.74 (15)	C9D—C10D—C11D—C1D	−55.53 (14)
C3B—C10B—C11B—C12B	−61.82 (17)	C3D—C10D—C11D—C12D	−63.49 (14)
C9B—C10B—C11B—C12B	−170.80 (13)	C9D—C10D—C11D—C12D	−173.23 (12)
O2B—C11B—C12B—C13B	70.68 (19)	O2D—C11D—C12D—C13D	65.14 (15)
C1B—C11B—C12B—C13B	−164.22 (16)	C1D—C11D—C12D—C13D	−168.51 (13)
C10B—C11B—C12B—C13B	−54.5 (2)	C10D—C11D—C12D—C13D	−57.86 (16)
C11B—C12B—C13B—C14B	−112.4 (3)	C11D—C12D—C13D—C14D	125.66 (18)
O1B—C8B—C15B—C16B	−67.00 (18)	O1D—C8D—C15D—C16D	−67.62 (16)
C7B—C8B—C15B—C16B	166.07 (14)	C7D—C8D—C15D—C16D	166.72 (14)
C9B—C8B—C15B—C16B	55.36 (19)	C9D—C8D—C15D—C16D	56.47 (18)
C8B—C15B—C16B—C17B	−123.2 (2)	C8D—C15D—C16D—C17D	−124.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O1A—H1AO···O2A	0.84	1.71	2.5163 (15)	160
O2A—H2AO···O1D	0.84	1.86	2.6727 (14)	161
O1B—H1BO···O1A	0.84	1.85	2.6198 (14)	151
O2B—H2BO···O1B	0.84	1.73	2.5356 (16)	160
O1C—H1CO···O2B	0.84	1.89	2.7297 (15)	175
O2C—H2CO···O1C	0.84	1.74	2.5446 (16)	161
O1D—H1DH···O2D	0.84	1.73	2.5318 (15)	160
O2D—H2DH···O2C	0.84	1.87	2.6984 (14)	170

Fig. 1


C4a
C5a
C3a
C6a
C17a
C14a
C2a
C9a
C10a
C16a
C15a
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C13a
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C7a
C1a
C12a
O1a
O2a

Fig. 2

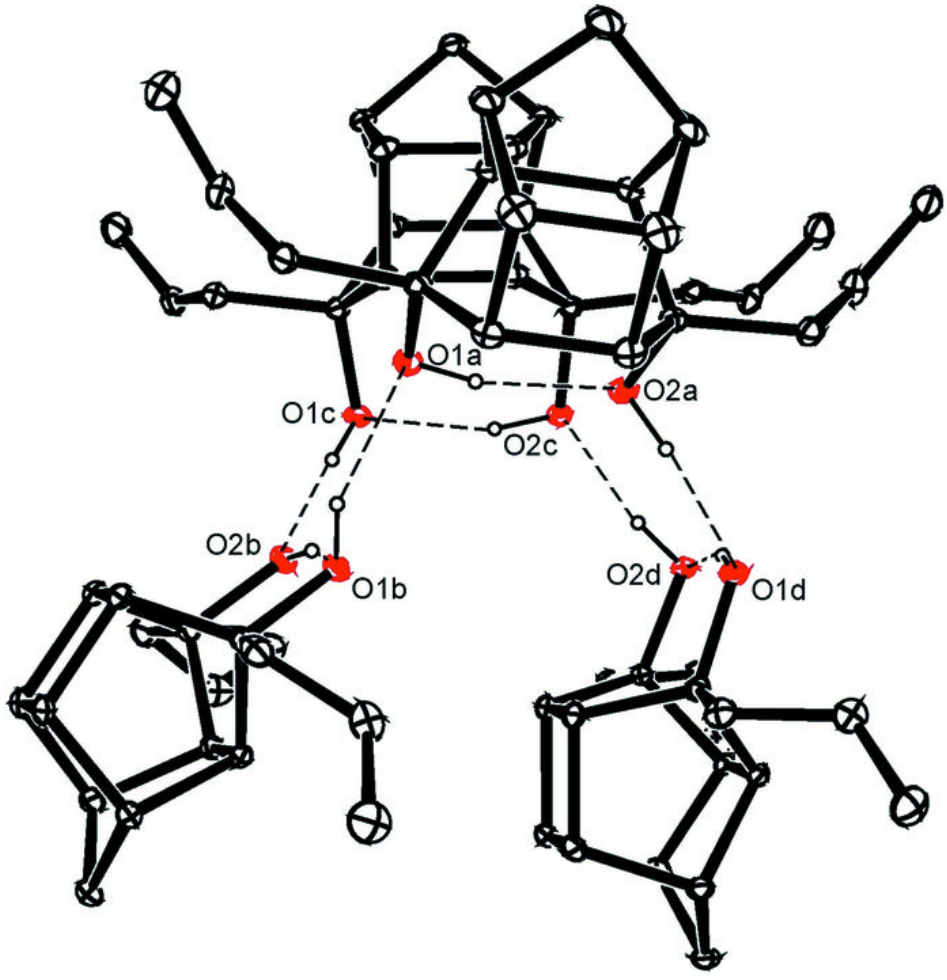

Fig. 3

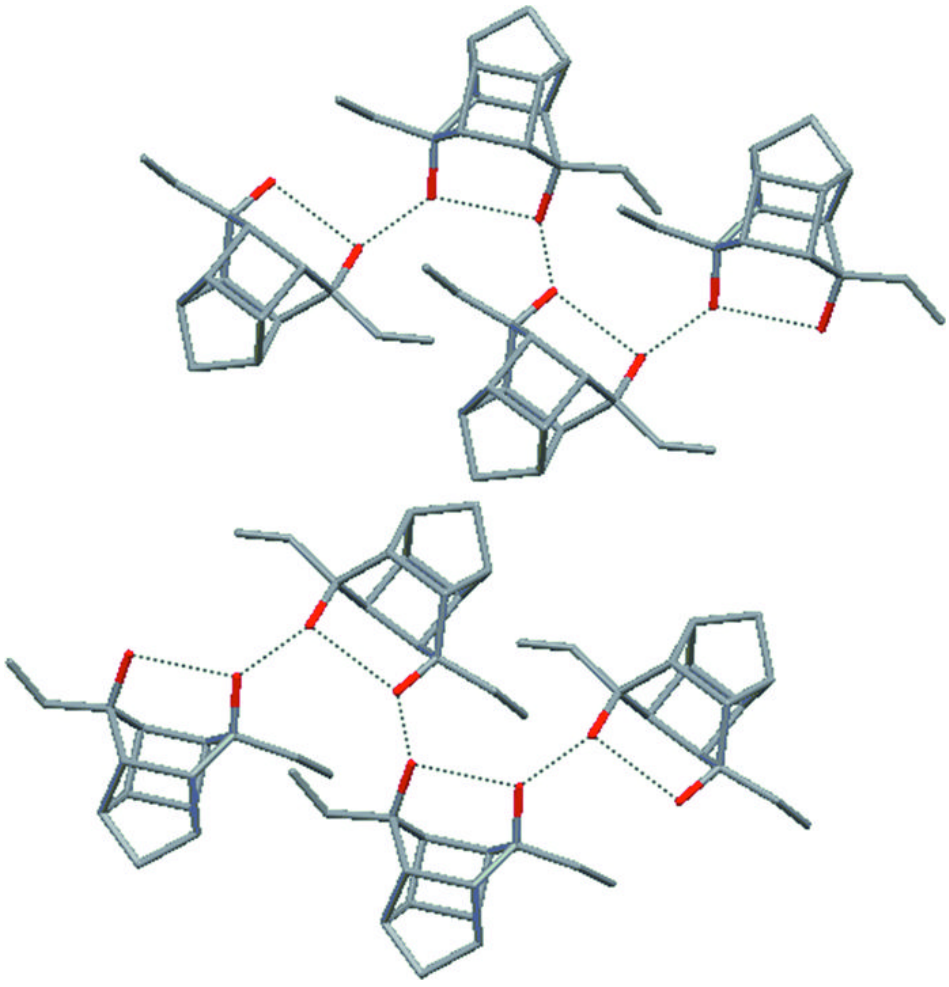

Fig. 4