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

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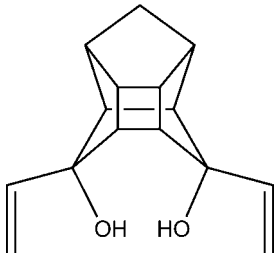
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 18.4.

The title molecule, $C_{15}H_{18}O_2$, exhibits C—C bond lengths that deviate from the normal value of 1.54 Å. A number of long [*e.g.* 1.5712 (16) Å] and short [*e.g.* 1.5237 (17) Å] C—C bonds are observed. The molecules are arranged in two-dimensional hydrogen-bonded (O—H···O) sheets with only hydrophobic van der Waals interactions between neighbouring sheets.

Related literature

For similar structures, see: Flippen-Anderson *et al.* (1991); Linden *et al.* (2005); Kruger *et al.* (2005, 2006).



Experimental

Crystal data

$C_{15}H_{18}O_2$
M_r = 230.29
Monoclinic, $P2_1/c$
a = 6.9355 (5) Å
b = 21.3303 (13) Å
c = 8.1859 (5) Å
β = 101.435 (3)°
V = 1186.95 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
0.48 × 0.40 × 0.34 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
15589 measured reflections
2869 independent reflections
2525 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.08
2869 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···O1	0.84	1.73	2.5409 (12)	160
O1—H1A···O2^{i}	0.84	1.85	2.6713 (11)	167

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART-NT* (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: FL2159).

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supplementary materials

Acta Cryst. (2007). E**63**, o3977 [**doi:10.1107/S1600536807042596**]

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

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

Comment

The title compound (**I**) consists of a large apolar (lipophilic) hydrocarbon skeleton with polar dihydroxy units (Fig. 1). This unique compound is used as a starting molecule and derivatives thereof are coupled with desired peptides as potential HIV-1 protease inhibitors. A number of publications have focused on the molecular geometries of pentacycloundecane (PCU) cage derivatives (Flippen-Anderson *et al.*, 1991; Linden *et al.*, 2005; Kruger *et al.*, 2005; Kruger *et al.*, 2006). It has been reported that these compounds exhibit bond lengths deviating from the normal value of 1.54 Å. The shortening and elongation of specific C—C bonds in the cage molecule is also observed in (i) with the C—C bonds between C3—C4 & C4—C5 being the shortest (1.5237 (17) Å & 1.5256 (17) Å respectively) and the bonds between C1—C7 & C1—C2 being the longest (1.5712 (16) Å & 1.5626 (16) Å respectively). Interestingly the bonds between the cage and the alkene side chains (C11—C12 and C8—C14) are surprisingly shorter than expected value of C—C bonds (1.54 Å) with values of 1.5173 (16) Å and 1.5212 (15) Å respectively. The ethylene chains are in an energetically favorable conformation, with atoms C8, C11, C12, C13, C14 coplanar. Atoms C13 and C15 appear to be in a *trans* conformation with respect to each other. This allows the two hydroxyl groups to be in a favorable conformation for intra- and intermolecular hydrogen bonding.

In (**I**)**,** the molecules pack in hydrogen-bonded bilayers. Both hydroxyl groups on the molecule participate in both intramolecular and intermolecular hydrogen bonding, each acting as a hydrogen bond donor and acceptor. Atom O2 interacts with atom O1 *via* H2A and atom O1 interacts with O2 of another cage molecule *via* H1A. Thus forming a hydrogen-bonded linear chain (Fig. 2). Because both the hydroxy groups of a molecule are involved in hydrogen bonding, molecules are connected in a linear fashion forming a sheet with alternating hydrogen bonding between the molecules. The linear sheets do not show any hydrogen bonding between the lipophilic parts of the bilayers but do show short contacts.

Experimental

A solution of Pentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,6}]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 vinylmagnesium 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 room temperature while stirring under nitrogen for 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 layer 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 (I) (27.0 g, 91%) as a colorless microcrystalline solid: m.p. 82–83 °C.

Refinement

All hydrogen atoms were first located in the difference map then positioned geometrically and allowed to ride on their respective parent atoms.

Figures

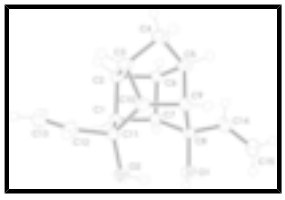

Fig. 1. The asymmetric unit of (I), showing the atomic numbering scheme and ellipsoids at the 50% probability level.

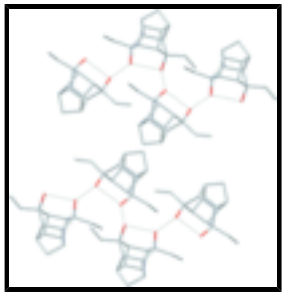

Fig. 2. Depiction of the intramolecular and intermolecular hydrogen bonding.

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

Crystal data

$C_{15}H_{18}O_2$	F_{000} = 496
M_r = 230.29	D_x = 1.289 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1016 reflections
a = 6.9355 (5) Å	θ = 3.6–28.3º
b = 21.3303 (13) Å	μ = 0.08 mm^{-1}
c = 8.1859 (5) Å	T = 173 (2) K
β = 101.435 (3)º	Irregular, colourless
V = 1186.95 (13) Å^3	0.48 × 0.40 × 0.34 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2525 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.031
Monochromator: graphite	θ_{max} = 28.0º
T = 173(2) K	θ_{min} = 1.9º
φ and ω scans	h = −9→9
Absorption correction: none	k = −28→28
15589 measured reflections	l = −10→10
2869 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
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.115$	$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 0.3441P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
2869 reflections	$\Delta\rho_{max} = 0.35$ e Å^{-3}
156 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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. 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 $F^2 > 2$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}
C1	0.93905 (16)	0.33993 (5)	0.24919 (14)	0.0231 (2)
H1	1.0523	0.3101	0.2724	0.028*
C2	0.99718 (17)	0.41041 (6)	0.23947 (15)	0.0269 (3)
H2	1.1400	0.4203	0.2495	0.032*
C3	0.85062 (18)	0.44024 (5)	0.09116 (15)	0.0273 (3)
H3	0.9047	0.4482	−0.0115	0.033*
C4	0.7748 (2)	0.49790 (6)	0.16851 (17)	0.0323 (3)
H4A	0.6623	0.5180	0.0934	0.039*
H4B	0.8794	0.5292	0.2072	0.039*
C5	0.71320 (18)	0.46260 (5)	0.31196 (15)	0.0275 (3)
H5	0.6537	0.4889	0.3903	0.033*
C6	0.90169 (17)	0.42568 (5)	0.39229 (15)	0.0264 (3)
H6	0.9882	0.4445	0.4925	0.032*
C7	0.84341 (16)	0.35538 (5)	0.40315 (14)	0.0225 (2)
H7	0.9050	0.3337	0.5090	0.027*
C8	0.61711 (16)	0.35801 (5)	0.36817 (13)	0.0208 (2)
C9	0.58290 (16)	0.40754 (5)	0.22715 (14)	0.0230 (2)
H9	0.4413	0.4196	0.1930	0.028*

C10	0.68068 (17)	0.39180 (5)	0.07136 (14)	0.0234 (2)
H10	0.5858	0.3964	−0.0372	0.028*
C11	0.79558 (16)	0.32932 (5)	0.08322 (14)	0.0220 (2)
C12	0.8997 (2)	0.32246 (6)	−0.06228 (16)	0.0306 (3)
H12	0.8182	0.3212	−0.1702	0.037*
C13	1.0912 (2)	0.31811 (7)	−0.0554 (2)	0.0420 (3)
H13A	1.1796	0.3192	0.0493	0.050*
H13B	1.1405	0.3139	−0.1552	0.050*
C14	0.54886 (18)	0.38205 (6)	0.52223 (15)	0.0281 (3)
H14	0.6216	0.4153	0.5823	0.034*
C15	0.3968 (2)	0.36033 (7)	0.57897 (16)	0.0339 (3)
H15A	0.3203	0.3270	0.5225	0.041*
H15B	0.3638	0.3780	0.6764	0.041*
O1	0.51761 (12)	0.30019 (4)	0.31854 (10)	0.02288 (19)
H1A	0.5584	0.2724	0.3898	0.034*
O2	0.67635 (13)	0.27405 (4)	0.07257 (10)	0.0267 (2)
H2A	0.6092	0.2750	0.1474	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0207 (5)	0.0224 (5)	0.0256 (5)	0.0012 (4)	0.0035 (4)	−0.0025 (4)
C2	0.0228 (5)	0.0253 (6)	0.0332 (6)	−0.0043 (4)	0.0069 (4)	−0.0040 (5)
C3	0.0337 (6)	0.0214 (5)	0.0291 (6)	−0.0037 (4)	0.0114 (5)	0.0022 (4)
C4	0.0400 (7)	0.0204 (5)	0.0381 (7)	−0.0016 (5)	0.0115 (5)	0.0027 (5)
C5	0.0333 (6)	0.0190 (5)	0.0319 (6)	0.0008 (4)	0.0104 (5)	−0.0009 (4)
C6	0.0278 (6)	0.0240 (5)	0.0268 (5)	−0.0054 (4)	0.0040 (4)	−0.0055 (4)
C7	0.0226 (5)	0.0226 (5)	0.0210 (5)	0.0003 (4)	0.0011 (4)	−0.0019 (4)
C8	0.0226 (5)	0.0190 (5)	0.0207 (5)	−0.0006 (4)	0.0040 (4)	−0.0001 (4)
C9	0.0222 (5)	0.0215 (5)	0.0254 (5)	0.0033 (4)	0.0053 (4)	0.0042 (4)
C10	0.0258 (5)	0.0229 (5)	0.0215 (5)	−0.0003 (4)	0.0046 (4)	0.0039 (4)
C11	0.0248 (5)	0.0200 (5)	0.0216 (5)	−0.0030 (4)	0.0054 (4)	−0.0012 (4)
C12	0.0399 (7)	0.0279 (6)	0.0267 (6)	−0.0051 (5)	0.0135 (5)	−0.0039 (5)
C13	0.0442 (8)	0.0430 (8)	0.0456 (8)	−0.0066 (6)	0.0256 (6)	−0.0098 (6)
C14	0.0329 (6)	0.0271 (6)	0.0249 (6)	0.0026 (5)	0.0075 (5)	−0.0014 (4)
C15	0.0337 (6)	0.0423 (7)	0.0275 (6)	0.0035 (5)	0.0102 (5)	−0.0013 (5)
O1	0.0263 (4)	0.0213 (4)	0.0204 (4)	−0.0038 (3)	0.0034 (3)	0.0019 (3)
O2	0.0356 (5)	0.0229 (4)	0.0232 (4)	−0.0089 (3)	0.0096 (3)	−0.0052 (3)

Geometric parameters (Å, °)

C1—C11	1.5333 (15)	C8—O1	1.4322 (13)
C1—C2	1.5626 (16)	C8—C14	1.5212 (15)
C1—C7	1.5712 (16)	C8—C9	1.5481 (15)
C1—H1	1.0000	C9—C10	1.5944 (15)
C2—C3	1.5565 (17)	C9—H9	1.0000
C2—C6	1.5614 (17)	C10—C11	1.5459 (15)
C2—H2	1.0000	C10—H10	1.0000
C3—C4	1.5237 (17)	C11—O2	1.4328 (13)

C3—C10	1.5516 (16)	C11—C12	1.5173 (16)
C3—H3	1.0000	C12—C13	1.322 (2)
C4—C5	1.5256 (17)	C12—H12	0.9500
C4—H4A	0.9900	C13—H13A	0.9500
C4—H4B	0.9900	C13—H13B	0.9500
C5—C6	1.5558 (17)	C14—C15	1.3177 (18)
C5—C9	1.5585 (16)	C14—H14	0.9500
C5—H5	1.0000	C15—H15A	0.9500
C6—C7	1.5601 (16)	C15—H15B	0.9500
C6—H6	1.0000	O1—H1A	0.8400
C7—C8	1.5396 (15)	O2—H2A	0.8400
C7—H7	1.0000		
C11—C1—C2	103.03 (9)	C6—C7—H7	115.0
C11—C1—C7	116.02 (9)	C1—C7—H7	115.0
C2—C1—C7	89.61 (8)	O1—C8—C14	108.29 (9)
C11—C1—H1	114.9	O1—C8—C7	115.95 (9)
C2—C1—H1	114.9	C14—C8—C7	109.35 (9)
C7—C1—H1	114.9	O1—C8—C9	112.47 (9)
C3—C2—C6	102.97 (9)	C14—C8—C9	111.18 (9)
C3—C2—C1	107.33 (9)	C7—C8—C9	99.41 (9)
C6—C2—C1	90.30 (9)	C8—C9—C5	101.10 (9)
C3—C2—H2	117.4	C8—C9—C10	115.21 (9)
C6—C2—H2	117.4	C5—C9—C10	102.36 (9)
C1—C2—H2	117.4	C8—C9—H9	112.4
C4—C3—C10	105.27 (10)	C5—C9—H9	112.4
C4—C3—C2	103.39 (10)	C10—C9—H9	112.4
C10—C3—C2	100.03 (9)	C11—C10—C3	101.31 (9)
C4—C3—H3	115.4	C11—C10—C9	115.28 (9)
C10—C3—H3	115.4	C3—C10—C9	102.17 (9)
C2—C3—H3	115.4	C11—C10—H10	112.4
C3—C4—C5	95.39 (9)	C3—C10—H10	112.4
C3—C4—H4A	112.7	C9—C10—H10	112.4
C5—C4—H4A	112.7	O2—C11—C12	103.39 (9)
C3—C4—H4B	112.7	O2—C11—C1	116.15 (9)
C5—C4—H4B	112.7	C12—C11—C1	112.55 (10)
H4A—C4—H4B	110.2	O2—C11—C10	114.93 (9)
C4—C5—C6	103.59 (10)	C12—C11—C10	110.69 (9)
C4—C5—C9	104.78 (10)	C1—C11—C10	99.46 (9)
C6—C5—C9	99.86 (9)	C13—C12—C11	127.17 (12)
C4—C5—H5	115.5	C13—C12—H12	116.4
C6—C5—H5	115.5	C11—C12—H12	116.4
C9—C5—H5	115.5	C12—C13—H13A	120.0
C5—C6—C7	107.76 (9)	C12—C13—H13B	120.0
C5—C6—C2	102.78 (9)	H13A—C13—H13B	120.0
C7—C6—C2	90.06 (8)	C15—C14—C8	125.17 (12)
C5—C6—H6	117.4	C15—C14—H14	117.4
C7—C6—H6	117.4	C8—C14—H14	117.4
C2—C6—H6	117.4	C14—C15—H15A	120.0
C8—C7—C6	102.74 (9)	C14—C15—H15B	120.0

C8—C7—C1	115.81 (9)	H15A—C15—H15B	120.0
C6—C7—C1	90.03 (8)	C8—O1—H1A	109.5
C8—C7—H7	115.0	C11—O2—H2A	109.5
C11—C1—C2—C3	12.86 (11)	C14—C8—C9—C5	60.93 (11)
C7—C1—C2—C3	−103.80 (9)	C7—C8—C9—C5	−54.18 (10)
C11—C1—C2—C6	116.56 (9)	O1—C8—C9—C10	−67.96 (12)
C7—C1—C2—C6	−0.10 (8)	C14—C8—C9—C10	170.41 (9)
C6—C2—C3—C4	33.62 (11)	C7—C8—C9—C10	55.30 (11)
C1—C2—C3—C4	128.07 (10)	C4—C5—C9—C8	151.87 (9)
C6—C2—C3—C10	−74.86 (10)	C6—C5—C9—C8	44.86 (10)
C1—C2—C3—C10	19.58 (11)	C4—C5—C9—C10	32.70 (11)
C10—C3—C4—C5	51.65 (11)	C6—C5—C9—C10	−74.31 (10)
C2—C3—C4—C5	−52.87 (11)	C4—C3—C10—C11	−151.85 (9)
C3—C4—C5—C6	52.79 (11)	C2—C3—C10—C11	−44.86 (10)
C3—C4—C5—C9	−51.46 (11)	C4—C3—C10—C9	−32.59 (11)
C4—C5—C6—C7	−127.37 (10)	C2—C3—C10—C9	74.39 (10)
C9—C5—C6—C7	−19.40 (11)	C8—C9—C10—C11	0.03 (13)
C4—C5—C6—C2	−33.14 (11)	C5—C9—C10—C11	108.76 (10)
C9—C5—C6—C2	74.83 (10)	C8—C9—C10—C3	−108.86 (10)
C3—C2—C6—C5	−0.27 (11)	C5—C9—C10—C3	−0.14 (10)
C1—C2—C6—C5	−108.14 (9)	C2—C1—C11—O2	−164.04 (9)
C3—C2—C6—C7	107.97 (9)	C7—C1—C11—O2	−68.00 (13)
C1—C2—C6—C7	0.10 (8)	C2—C1—C11—C12	77.06 (11)
C5—C6—C7—C8	−13.17 (11)	C7—C1—C11—C12	173.10 (9)
C2—C6—C7—C8	−116.62 (9)	C2—C1—C11—C10	−40.14 (10)
C5—C6—C7—C1	103.35 (9)	C7—C1—C11—C10	55.90 (11)
C2—C6—C7—C1	−0.10 (8)	C3—C10—C11—O2	178.71 (9)
C11—C1—C7—C8	−0.04 (14)	C9—C10—C11—O2	69.30 (12)
C2—C1—C7—C8	104.29 (10)	C3—C10—C11—C12	−64.64 (11)
C11—C1—C7—C6	−104.24 (10)	C9—C10—C11—C12	−174.05 (9)
C2—C1—C7—C6	0.10 (8)	C3—C10—C11—C1	53.96 (10)
C6—C7—C8—O1	161.29 (9)	C9—C10—C11—C1	−55.45 (11)
C1—C7—C8—O1	64.97 (12)	O2—C11—C12—C13	−118.34 (14)
C6—C7—C8—C14	−75.97 (11)	C1—C11—C12—C13	7.78 (18)
C1—C7—C8—C14	−172.29 (9)	C10—C11—C12—C13	118.09 (15)
C6—C7—C8—C9	40.53 (10)	O1—C8—C14—C15	−12.52 (16)
C1—C7—C8—C9	−55.78 (11)	C7—C8—C14—C15	−139.71 (13)
O1—C8—C9—C5	−177.44 (9)	C9—C8—C14—C15	111.52 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2A···O1	0.84	1.73	2.5409 (12)	160
O1—H1A···O2^{i}	0.84	1.85	2.6713 (11)	167

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2.

Fig. 1

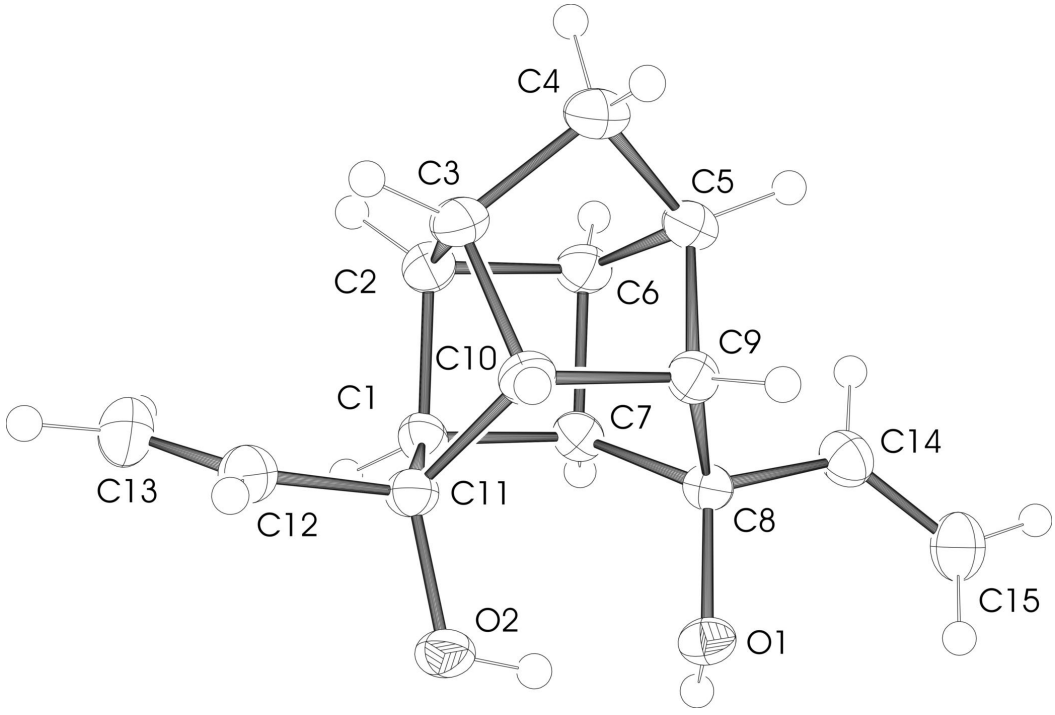

Fig. 2