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Adamantane-1,2-diol

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In the crystal structure of the title compound, $C_{10}H_{16}O_2$, the hydroxyl groups are involved in both intra- and intermolecular hydrogen bonding. Molecules are arranged in discrete layers propagated by a network of O—H···O hydrogen-bonding interactions. The asymmetric unit comprises one chiral molecule but the presence of a crystallographic centre of inversion leads to racemic crystals.

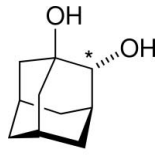
Key indicators

Single-crystal X-ray study
T = 83 K
Mean σ(C–C) = 0.002 Å
R factor = 0.061
wR factor = 0.176
Data-to-parameter ratio = 26.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Being a rigid cage-like molecule with two substituents which are capable of hydrogen bonding, adamantane-1,2-diol, (I), promises to be an interesting candidate as a template for molecular imprinting. There is a chiral centre at position C-2; however, the title compound crystallizes as the racemate.



(I)

The molecular structure of (I) is illustrated in Fig. 1. In the molecule, there is an intramolecular hydrogen bond

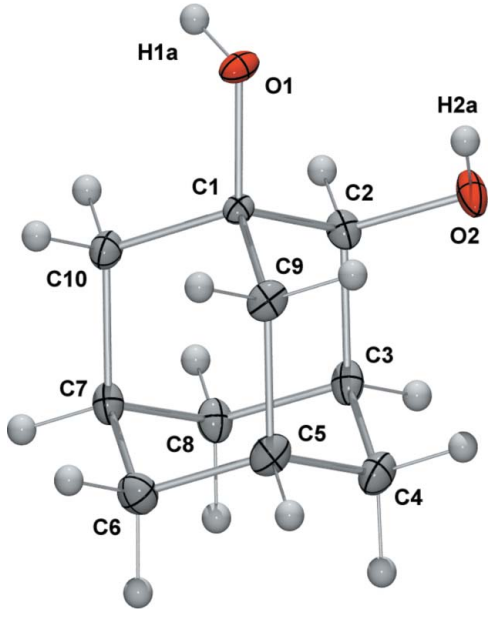


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level and H atoms shown as spheres of arbitrary radii.

[O2···O1 = 2.8688 (15) Å]. In the crystal structure (Fig. 2), molecules are arranged in discrete two-dimensional layers that lie parallel to the crystallographic *ac* plane. Intermolecular hydrogen-bonding interactions (Table 1) form a two-dimensional scaffold supporting bilayers of molecules of (I).

Experimental

Adamantane-1,2-diol was synthesized *via* a four-step synthesis according to the methods of McKervey *et al.* (1971) and Janjatovic *et al.* (1980). After repeated recrystallization from methanol at room temperature, colourless block-shaped crystals of (I) were obtained.

Crystal data

$C_{10}H_{16}O_2$
M_r = 168.23
Orthorhombic, *Pccn*
a = 9.6159 (3) Å
b = 20.6781 (7) Å
c = 8.3921 (2) Å
V = 1668.67 (9) Å^3
Z = 8
D_x = 1.339 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2252 reflections
θ = 3.4–32.6°
μ = 0.09 mm^{-1}
T = 83 (2) K
Block, colourless
0.36 × 0.24 × 0.10 mm

Data collection

Bruker Kappa-APEX-II area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.684, T_{max} = 1.000
41081 measured reflections
2845 independent reflections
2252 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 32.7°
$h = -13 \rightarrow 13$
$k = -30 \rightarrow 31$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.176
S = 1.03
2845 reflections
109 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0791P)^2 + 1.9937P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 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	2.45	2.8688 (15)	112
O1—H1A···O2^{i}	0.84	2.02	2.8625 (15)	176
O2—H2A···O1^{ii}	0.84	2.10	2.8633 (14)	152

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

H atoms were included in idealized positions and refined using a riding model, with tertiary and secondary C—H bond lengths fixed at 0.99 and 1.00 Å, respectively, and the O—H bonds fixed at 0.84 Å. U_{iso}(H) values were fixed at 1.2U_{eq} of the parent C and O atoms.

Data collection: *APEXII* (Bruker 2004); cell refinement: *APEXII* and *SAINT* (Bruker 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *POV-RAY* (Persistence of Vision, 2004); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

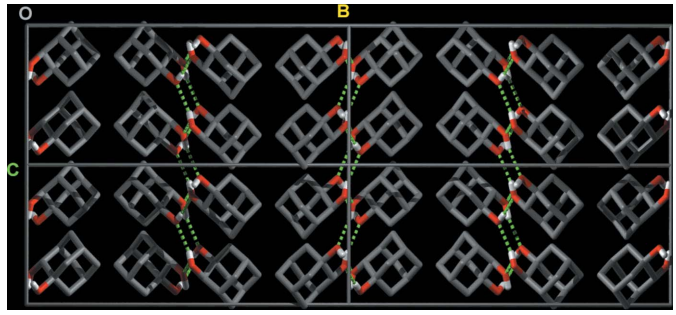


Figure 2
Crystal packing diagram of (I), viewed along the *a* axis. Key: C grey, H white and O red. Hydrogen bonds are shown as green dashed lines (H atoms not involved in hydrogen bonding have been omitted for clarity). The molecules are arranged in layers parallel to the *ac* plane.

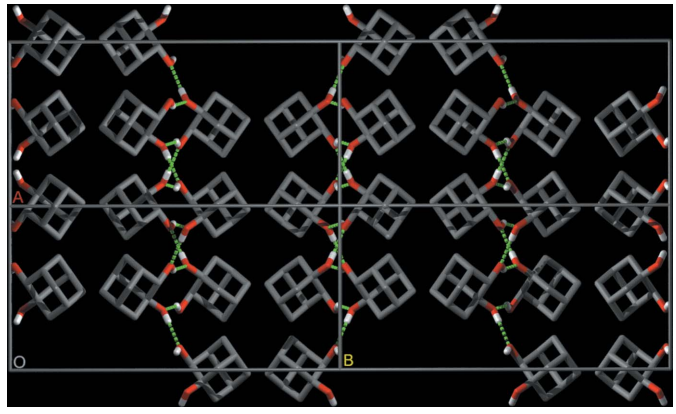


Figure 3
Crystal packing diagram of (I), viewed along the *c* axis. Key: C grey, H white and O red. Hydrogen bonds are shown as green dashed lines (H atoms not involved in hydrogen bonding have been omitted for clarity). The molecules are arranged in layers parallel to the *ac* plane.

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