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1-Hydroxydiamantane

Chu-Yi Yu,[a]* Qian Li,[a,b] Li-Ben Wang[a] and Hong-Wei Ma[c]

[a]Beijing National Laboratory for Molecular Science (BNLMS), Laboratory for Chemical Biology, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, People's Republic of China, [b]College of Chemistry and Molecular Sciences, University of Wuhan, Wuhan 453000, People's Republic of China, and [c]Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, People's Republic of China

Correspondence e-mail: yucy@iccas.ac.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.149
Data-to-parameter ratio = 17.9

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

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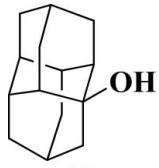
The molecule of the title compound, $C_{14}H_{20}O$, posseses normal geometrical parameters. The compound crystallizes in the uncommon space group $P4_2/n$ and features discrete quartets of molecules linked by O—H···O bonds into a loop.

Comment

The title compound, (I) (Fig. 1), is a derivative of diamantane. Diamantane is a member of the diamondoid family: a hydrocarbon that has a carbon framework that is superimposable on the diamond lattice. Diamantane derivatives are potentially valuable molecules both in materials science and in pharmaceutical sciences. For example, (I) is an intermediate for the synthesis of a variety of other diamantane derivatives such as 1-bromodiamantane, 1-aminodiamantane and 1-diamantanecarboxylic acid.



(I)

The geometrical parameters for (I) are normal. The crystal structure is stabilized by intermolecular O—H···O hydrogen bonds (Table 1), which result in the formation of discrete quartets (Figs. 2 and 3) of molecules.

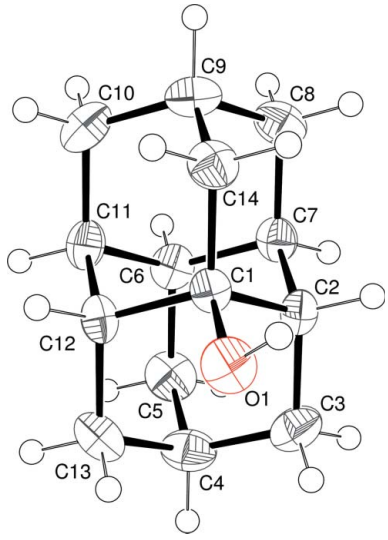


Figure 1
View of (I), showing 50% displacement ellipsoids (arbitrary spheres for H atoms).

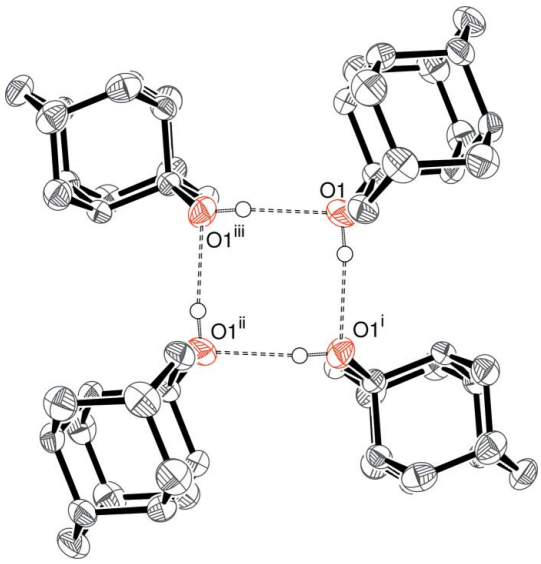


Figure 2
View of a quartet of molecules linked by hydrogen bonds (50% displacement ellipsoids) C-bound H atoms have been omitted for clarity and hydrogen bonds are shown as dashed lines. [Symmetry codes: (i) $\frac{1}{2}-y, x, \frac{1}{2}-z$; (ii) $\frac{1}{2}-x, \frac{1}{2}-y, z$; (iii) $y, \frac{1}{2}-x, \frac{1}{2}-z$.]

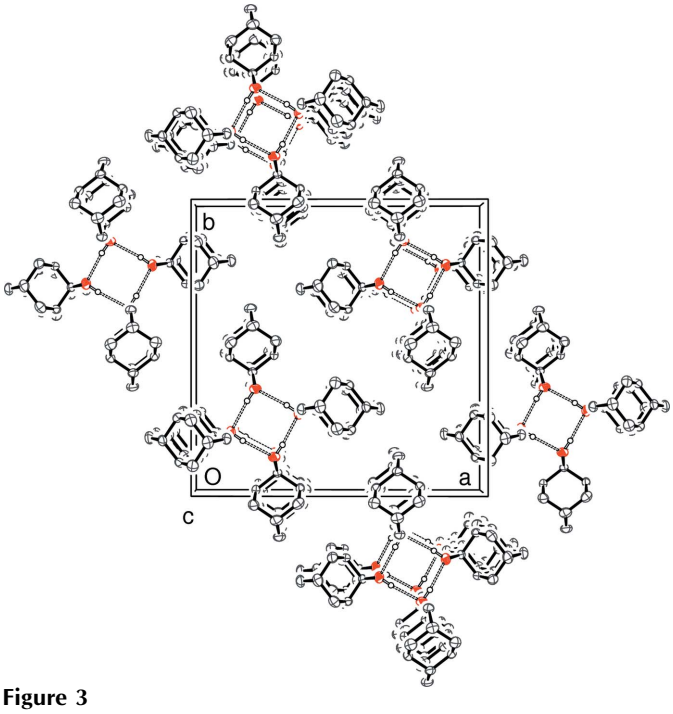


Figure 3
: The packing of (I). Drawing conventions as in Fig. 2.

Experimental

The title compound was prepared according to the procedure reported by Fokin *et al.* (2005) in 69.4% yield. Suitable crystals were recrystallized from acetone (m.p. 564–565 K). ^{13}C NMR ($CDCl_3$, 75 MHz): δ 70.72 (1C, C-1), 46.33 (1C, C-14), 43.31 (2C, C-2, C-12), 39.88 (2C, C-7, C-11), 37.92 (1C, C-5), 37.46 (2C, C-8, C-10), 36.66 (1C, C-6), 32.47 (2C, C-3, C-13), 30.37 (1C, C-9), 25.23 (1C, C-4). Analysis calculated for $C_{14}H_{20}O$: C 82.30, H 9.87%; found: C 82.34, H 9.80%.

Crystal data

$C_{14}H_{20}O$
M_r = 204.30
Tetragonal, $P4_2/n$
a = 16.572 (2) Å
c = 7.7879 (16) Å
V = 2138.8 (6) Å^3
Z = 8
D_x = 1.269 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
Prism, colorless
0.64 × 0.22 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.952, T_{max} = 0.986
18440 measured reflections
2441 independent reflections
1899 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.149
S = 1.05
2441 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O1^{i}	0.82	1.96	2.7581 (13)	166

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

All H atoms were initially located in a difference Fourier map. There were repositioned with ideal geometry (C—H = 0.97–0.98 Å and O—H = 0.82 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier).

Data collection: *RAPID-AUTO* (Rigaku, 2001); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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