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2,2,6,6-Tetramethylpiperidin-4-ol

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Key indicators

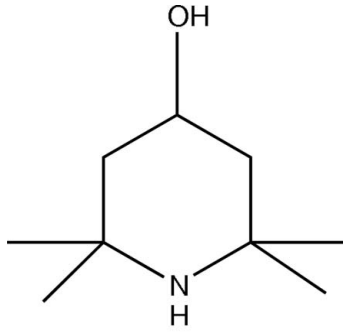
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.052
wR factor = 0.120
Data-to-parameter ratio = 17.0

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

The molecule of the title compound, $C_9H_{19}NO$, lies on a mirror plane. Intermolecular N—H···O and O—H···N hydrogen bonds are observed in the crystal structure.

Comment

2,2,6,6-Tetramethyl-piperidin-4-ol, (I), is an important compound, since it represents a key intermediate in the preparation of stable nitroxyl radicals, such as 4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl and 4-amino-2,2,6,6-tetramethylpiperidine-1-oxyl, which are used in spin-labeling medicinal studies (Sinha *et al.*, 1979) and as efficient photo-stabilizing agents for plastic products (Bellus *et al.*, 1972).



(I)

We present the X-ray crystallographic analysis of (I) (Fig. 1). The molecule lies on a mirror plane, with atoms N1,

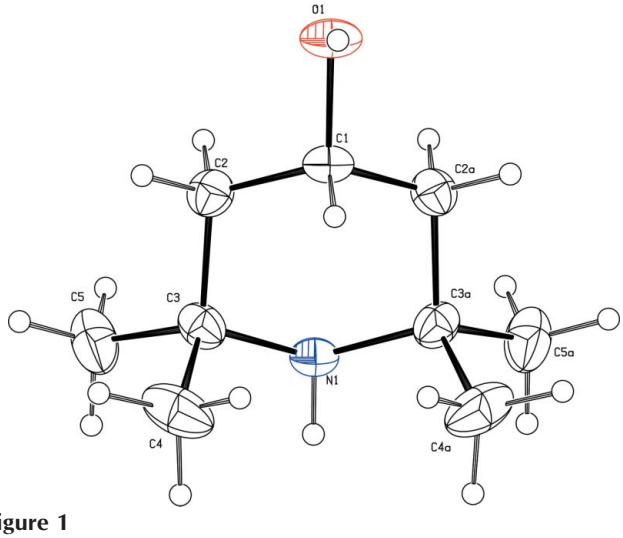


Figure 1
A drawing of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (*a*) $-x, y, z$.]

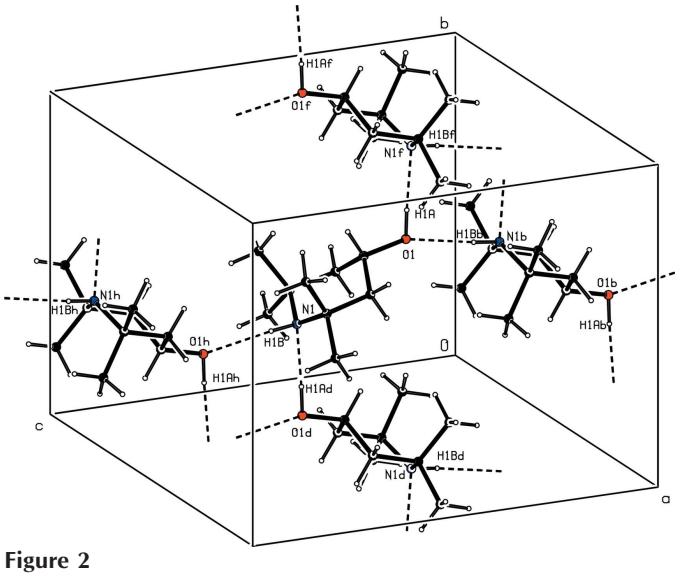


Figure 2
The crystal packing of (I). Dashed lines indicate hydrogen bonds. [Symmetry codes: (*b*) $-x, \frac{1}{2}-y, -\frac{1}{2}+z$; (*d*) $x, -\frac{1}{2}+y, \frac{3}{2}+z$; (*f*) $x, y-\frac{1}{2}, -z+\frac{3}{2}$; (*h*) $-x, -y+\frac{1}{2}, z+\frac{1}{2}$.]

H1*B*, C1, H1, O1 and H1*A* on special positions (0,*y*,*z*). The bond lengths and angles are unexceptional. As shown in Fig. 2 and Table 1, N—H···O and O—H···N intermolecular hydrogen bonds link the molecules.

Experimental

The title compound was synthesized according to the procedure of Lutz *et al.* (1962). Crystals suitable for data collection were obtained by slow evaporation of a chloroform solution at 283 K.

Crystal data

$C_9H_{19}NO$
$M_r = 157.25$
Orthorhombic, *Cmca*
$a = 14.149\ (2)$ Å
$b = 10.1346\ (15)$ Å
$c = 13.3806\ (18)$ Å
$V = 1918.7\ (5)$ Å^3
$Z = 8$
$D_x = 1.089$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 635 reflections
$\theta = 2.9$–$21.6°$
$\mu = 0.07$ mm^{-1}
$T = 292\ (2)$ K
Block, colorless
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
4310 measured reflections
1091 independent reflections
627 reflections with $I > 2\sigma(I)$
$R_{int} = 0.093$
$\theta_{max} = 27.0°$
$h = -15 \rightarrow 18$
$k = -12 \rightarrow 11$
$l = -14 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.120$
$S = 0.88$
1091 reflections
64 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0144 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O1^{i}	0.85 (2)	2.28 (2)	3.132 (3)	177 (2)
O1—H1A···N1	0.91 (3)	1.99 (3)	2.904 (2)	178 (3)

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

H atoms bonded to N and O atoms were located in a difference map and refined with $U_{iso}(H) = 1.2U_{eq}(N)$ and $U_{iso}(H) = 1.5U_{eq}(O)$. Bond lengths were constrained to N—H = 0.85 Å and O—H = 0.91 Å. H atoms bonded to C atoms were placed in calculated positions and treated as riding on their parent atoms, with displacement parameters fixed at $U_{iso} = 1.5U_{eq}$(carrier atom) for methine and methyl groups, and $U_{iso} = 1.2U_{eq}$(carrier atom) for methylene groups. Bond lengths were constrained to 0.96 (methyl CH_3), 0.97 (methylene CH_2) or 0.98 Å (methine CH).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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