organic papers

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Key indicators

Single-crystal X-ray study
$T = 150$ K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.117
Data-to-parameter ratio = 19.2

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

3-Ethylpentan-3-ol

The crystal structure of the title compound, $C_7H_{16}O$, has been determined at 150 (2) K following *in situ* crystal growth from the liquid. The structure contains four independent molecules in the asymmetric unit, forming a fourfold cyclic arrangement *via* O—H···O hydrogen bonds.

Comment

Just over a decade ago, Brock & Duncan (1994) noted that monoalcohols commonly crystallize in high-symmetry space groups (tetragonal, trigonal, hexagonal and cubic groups) or with more than one independent molecule in the asymmetric unit ($Z' > 1$). This can be rationalized by considering that the geometrical features of extended O—H···O hydrogen-bond motifs are rarely compatible with efficient packing of the molecules about 2_1 screw axes or glide planes, or by simple translation. The crystal structure of the title compound, (I), is a typical example; the asymmetric unit in space group $P\bar{1}$ comprises a fourfold cyclic arrangement formed *via* O—H···O hydrogen bonds (Fig. 1 and Table 1). These units are arranged in approximate hexagonal close-packed layers, which stack directly one upon the other to form a simple hexagonal arrangement in three dimensions (Fig. 2).
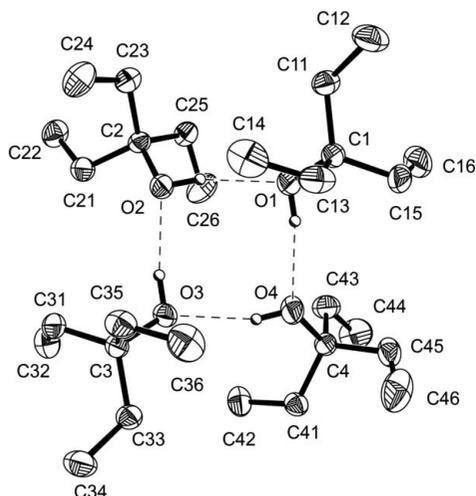

(I)
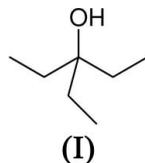
Experimental

Compound (I) (98%) was obtained from the Aldrich Company and was used without further purification. The crystal was grown in a 0.4 mm glass capillary tube using a technique described previously (Davies & Bond, 2001), at *ca* 258 K (a temperature only slightly less than the melting point of the solid in the capillary tube). Once formed, the crystal was cooled slowly to 150 K for data collection. The length of the cylindrical crystal could not be estimated accurately, but it exceeded the diameter of the collimator (0.60 mm).

Crystal data

$C_7H_{16}O$	$V = 1556.1$ (2) Å^3
$M_r = 116.20$	$Z = 8$
Triclinic, $P\bar{1}$	$D_x = 0.992$ Mg m^{-3}
$a = 10.5552$ (10) Å	Mo $K\alpha$ radiation
$b = 11.2140$ (9) Å	$\mu = 0.06$ mm^{-1}
$c = 14.1681$ (13) Å	$T = 150$ (2) K
$\alpha = 88.682$ (3)°	Cylinder, colourless
$\beta = 72.512$ (3)°	0.60×0.20 (radius) mm
$\gamma = 76.904$ (4)°	

Figure 1
The asymmetric unit, showing displacement ellipsoids at the 50% probability level. H atoms bound to C atoms have been omitted. Dashed lines denote O—H···O hydrogen bonds.

Figure 2
Projection of the structure along the *a* axis, showing the approximate hexagonal close-packed arrangement of the fourfold hydrogen-bonded units. H atoms have been omitted.

Data collection

Bruker–Nonius X8APEX-II CCD diffractometer	apparent transmission: 0.711045
ω and φ scans	$T_{min} = 0.693$, $T_{max} = 0.975$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003); ratio of minimum to maximum	35248 measured reflections
	5870 independent reflections
	4402 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.049$
	$\theta_{max} = 25.8°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.044$	$+ 0.3995P]$
$wR(F^2) = 0.117$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
5870 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
305 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O4	0.84 (2)	1.98 (2)	2.7977 (16)	167.7 (18)
O2—H2···O1	0.86 (2)	1.93 (2)	2.7686 (14)	165.8 (17)
O3—H3···O2	0.87 (2)	1.92 (2)	2.7759 (15)	169.4 (18)
O4—H4···O3	0.81 (2)	2.01 (2)	2.7888 (15)	160.5 (18)

H atoms bound to C atoms were positioned geometrically and allowed to ride during subsequent refinement, with C—H = 0.99 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for the methylene groups, and C—H = 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl groups. The H atoms of the hydroxy groups were located in difference Fourier maps and refined without restraint, employing isotropic displacement parameters.

Data collection: *APEX2* (Bruker Nonius, 2004); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Brock, C. P. & Duncan, L. L. (1994). *Chem. Mater.* **6**, 1307–1312.
Bruker (2003). *SAINT*. Version 7.06a. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker Nonius (2004). *APEX2*. Version 1.0-22. Bruker Nonius BV, Delft, The Netherlands.
Davies, J. E. & Bond, A. D. (2001). *Acta Cryst.* E**57**, o947–o949.
Sheldrick, G. M. (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.