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Durenedimethanol

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Durenedimethanol (2,3,5,6-tetramethyl-1,4-phenylenedimethanol), $C_{12}H_{18}O_2$, crystallizes in space group $I4_1/a$ with a three-dimensional structure held together by O—H···O hydrogen bonds. The hydrogen bonds have a fourfold helical arrangement. The molecule lies on a crystallographic center of symmetry.

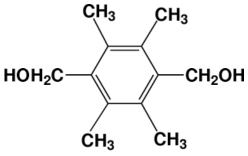
Key indicators

Single-crystal X-ray study
T = 174 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.104
Data-to-parameter ratio = 14.1

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

Comment

Shan & Jones (2001) have reported the structure of 1,4-benzenedimethanol, a molecule of potential use in crystal engineering. The structure of the durene analog, durenedimethanol, (I), is reported here.



(I)

The labeling and the anisotropic displacement parameters are shown in Fig. 1. The molecule lies on a crystallographic center of symmetry. The bond lengths and angles are normal. The ring is planar within experimental error [displacements (Å): C1 −0.001 (1), C2 0.001 (1), C3 0.001 (1)], but the substituents are distinctly puckered [displacements: C4 −0.108 (1), C5 0.108 (1), C6 −0.052 (1)]. These displacements are similar to those in hexamethylbenzene (Le MaguèRes *et al.*, 2001).

The packing is shown in Fig. 2. A 4_1 screw axis of hydrogen bonds can be clearly seen. The distances and angles in the hydrogen bonds are given in Table 1, where they are compared with those in benzenedimethanol (Shan & Jones, 2001) and benzenediisopropanol (Koritsánszky & Menczel, 1982). All of the individual hydrogen-bond parameters in durenedimethanol and benzenedimethanol are virtually identical. The benzenediisopropanol has O—H···O angles that are further from linear and slightly longer O···O distances. For discussions of hydrogen bonding in alcohols, see Brock & Duncan (1994) and Brock (2002).

The packings in the three structures are quite different. In all three, the graph sets (Etter *et al.*, 1990; Bernstein *et al.*, 1995) for the dominant interactions are the same, $C(2)$, if we consider all chemically equivalent OH groups to be the same. However, in benzenedimethanol adjacent OH groups in the chain are crystallographically independent so that an alternative description would be $C_2^2(4)$; together they form a pseudo-twofold screw axis. In benzenediisopropanol three adjacent OH groups in the chain are crystallographically

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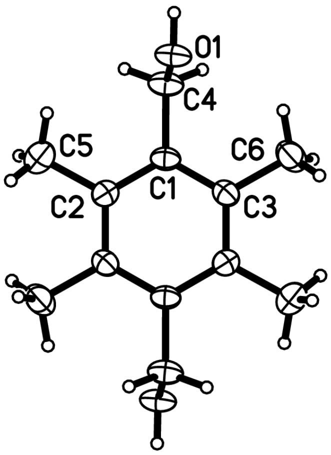

Figure 1
A view of the molecule of (I), with displacement ellipsoids drawn at the 50% probability level. The unlabeled atoms are related to the labeled atoms by a center of symmetry.

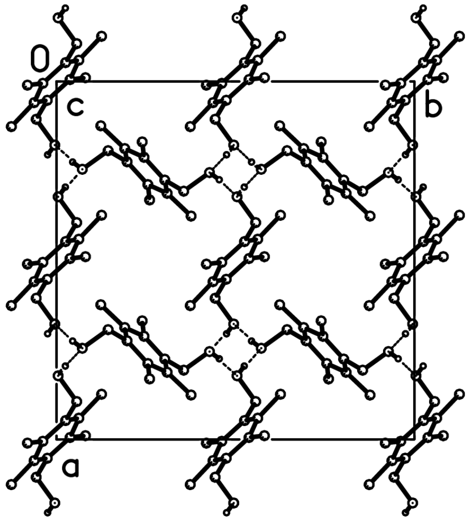

Figure 2
A view of the structure of (I) along the c axis. Hydrogen bonds are shown as dashed lines. Methyl and methylene H atoms have been omitted for clarity.

independent and the alternative description would be $C_3^3(6)$; together they form a pseudo-threefold screw axis. In durenedimethanol there is only one OH in the asymmetric unit, which is involved in interactions *via* a crystallographic fourfold screw axis.

If we return to considering the chemically equivalent OH groups the same, so that the basic graph sets are the same, the complex graph sets show the differences clearly: benzenedimethanol $C(2)[C(9)][R_4^4(22)]$, benzenediisopropanol $C(2)$-$[C(9)][R_2^2(18)][R_6^6(26)]$ and durenedimethanol $C(2)[R_4^4(36)$. In the first two, the overall hydrogen bonding leads to two-dimensional networks, while in durenedimethanol it leads to a three-dimensional network.

Finally, it should be noted that durenedimethanol and its isomer dimethoxydurene (Wieczorek *et al.*, 1975) have the same molecular volumes within experimental error despite the great differences in their intermolecular interactions and packing.

Experimental

The compound was obtained from the Shell Development Co. Satisfactory crystals grew as prisms from ethanol.

Crystal data

$C_{12}H_{18}O_2$
$M_r = 194.26$
Tetragonal, $I4_1/a$
$a = 16.042$ (4) Å
$c = 8.656$ (2) Å
$V = 2227.6$ (9) Å^3
$Z = 8$
$D_x = 1.159$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3471 reflections
$\theta = 2.5$–25.0°
$\mu = 0.08$ mm^{-1}
$T = 174$ (2) K
Prism, colorless
0.38 × 0.22 × 0.22 mm

Data collection

Siemens SMART area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
$T_{\min} = 0.97$, $T_{\max} = 0.98$
5239 measured reflections
990 independent reflections
871 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\max} = 25.1°$
$h = -19 \rightarrow 13$
$k = -18 \rightarrow 19$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.104$
$S = 1.13$
990 reflections
70 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 1.83P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}

Table 1
Distances and angles (Å,°) in the O—H···O hydrogen bonds.

O	H	O	O—H	O—H···O	H···O	H···O—C	C···O	Ref.
O1	H1	O1$^{\rm i}$	0.87 (2)	175 (2)	1.85 (2)	120 (2)	2.717 (2)	*a*
O1	H1	O2	0.90 (3)	174 (2)	1.82 (3)	119 (2)	2.714 (2)	*b*
O2	H2	O1	0.92 (2)	170 (2)	1.81 (3)	123 (2)	2.725 (2)	*b*
O1	H1	O3	1.07 (4)	155 (3)	1.75 (4)	124 (3)	2.757 (4)	*c*
O3	H3	O2	0.97 (4)	161 (3)	1.84 (4)	125 (3)	2.779 (4)	*c*
O2	H2	H1	0.97 (4)	156 (3)	1.93 (4)	124 (3)	2.848 (4)	*c*

Symmetry code: (i) $\frac{3}{4} - y, \frac{1}{4} + x, \frac{1}{4} + z$. References: (*a*) durenedimethanol (this work); (*b*) benzenedimethanol (Shan & Jones, 2001); (*c*) benzenediisopropanol (Koritsánszky & Menczel, 1982).

The methyl and methylene H atoms were included at idealized positions, with the methyl groups allowed to rotate around the C—C bonds. The hydroxy H atom was refined with an isotropic displacement parameter. The C—H distances were fixed at 0.99 Å for methylene and 0.98 Å for methyl H atoms. The isotropic displacement parameters for both were fixed at 1.5 times the $U_{\rm eq}$ value of the attached C atom.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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