Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

2,2′-Ethylidenebis(4-methylphenol)

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Received 16 March 2007
Accepted 30 March 2007

Key indicators

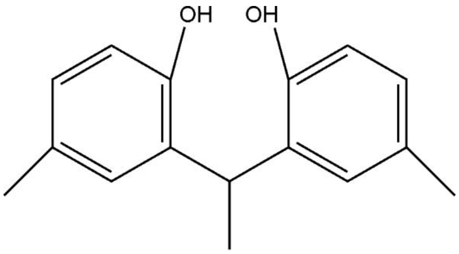
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.126
Data-to-parameter ratio = 9.4

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

In the molecule of the title compound, $C_{16}H_{18}O$, the dihedral angle between the rings is 70.61 (3)°. In the crystal structure, intermolecular O—H⋯O hydrogen bonds link the molecules into chains, and may be effective in the stabilization of the structure.

Comment

Bisphenol is useful as a starting material for the production of polycarbonate, polyester and epoxy resins, and as a modifier and stabilizer for phenol resins (Raymond *et al.*, 1958). We report here the crystal structure of the title compound, (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings *A* (C2–C7) and *B* (C10–C15) are, of course, planar and the dihedral angle between them is 70.61 (3)°.

As can be seen from the packing diagram (Fig. 2), the molecules of (I) are linked by intermolecular O—H⋯O hydrogen bonds (Table 1), forming infinite chains along the [010] direction, and they are stacked along the *a* axis. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

4-Methylphenol (108 g, 1 mol) was placed in a four-necked round-bottomed flask fitted with a mechanical stirrer, dropping funnel, thermometer and reflux condenser, and was dissolved in toluene (50 ml). The system was put in a water bath at 333 K and stirred for 30 min. Gaseous HCl was passed through the mixture for 30 min, and then paraldehyde (AR) (0.03 mol, 4.5 ml) was added and the mixture stirred. The reaction was maintained at 333 K in a water bath for 6 h. The mixture was washed with saturated aqueous sodium hydrogen carbonate (7.4%, 200 ml) and distilled water (200 ml). The starting material and solvent were distilled under reduced pressure. The product was purified by repeated crystallization. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethyl alcohol (AR) solution (95%, 10 ml) (yield 17.424 g, 72%; m.p. 663.8 K)

doi:10.1107/S1600536807015607

Crystal data

$C_{16}H_{18}O_2$
$M_r = 242.30$
Orthorhombic, $P2_12_12_1$
$a = 8.6680\ (17)$ Å
$b = 9.6400\ (19)$ Å
$c = 16.424\ (3)$ Å
$V = 1372.4\ (5)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 298\ (2)$ K
0.30 × 0.30 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.964$, $T_{\max} = 0.985$
1571 measured reflections
1555 independent reflections
1142 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.015$
3 standard reflections every 200 reflections intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.126$
$S = 1.08$
1555 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.13$ e Å^{-3}
Absolute structure: Flack (1983), 1121 Friedel pairs
Flack parameter: 0.03 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.82	1.92	2.725 (3)	168
O1—H1···O2$^{\rm i}$	0.82	1.97	2.766 (3)	165

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

H atoms were positioned geometrically [O—H = 0.82 Å, and C—H = 0.93, 0.98 and 0.96 Å for aromatic, methine and methyl H atoms, respectively] and constrained to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = xU_{\rm eq}({\rm C,O})$, where $x = 1.5$ for methyl and $x = 1.2$ for all other H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank Professor Hua-qin Wang of the Analysis Centre, Nanjing University, for help with the X-ray crystallographic analysis.

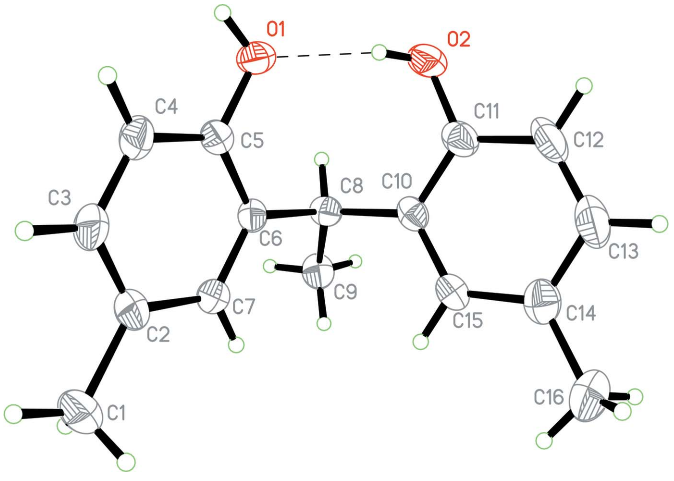


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular hydrogen bond is shown as a dashed line.

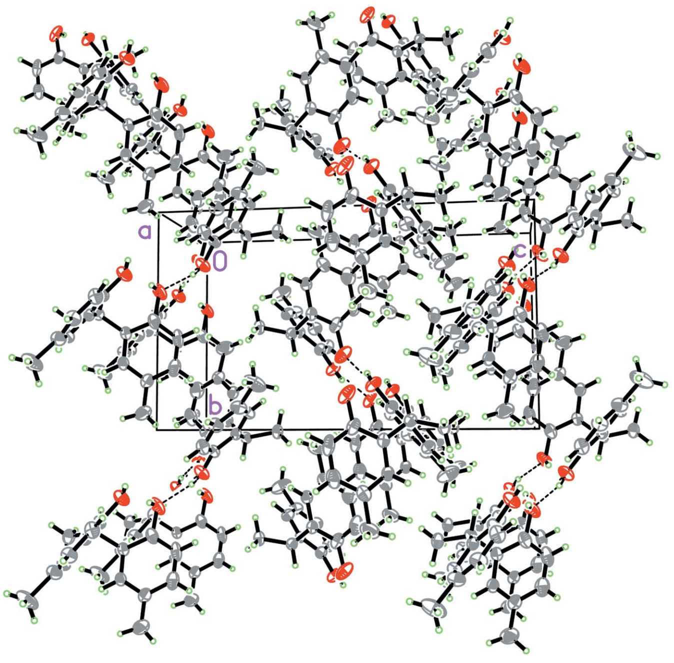


Figure 2
A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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