

2,4'-Isopropylidenediphenol

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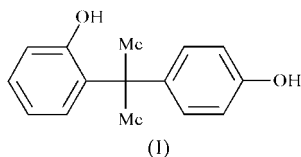
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Molecules of the title compound [systematic name: 2,4'-(propane-2,2-diyl)diphenol], C₁₅H₁₆O₂, are linked through intermolecular O—H...O hydrogen bonds into infinite zigzag chains. The molecular structure is compared with that of the related compound 4,4'-isopropylidenediphenol.

Comment

4,4'-Isopropylidenediphenol (commonly referred to as bisphenol-A or *p,p*-BPA), synthesized industrially by condensing phenol with acetone in the presence of an acid catalyst, is widely used as a basic material for the production of polycarbonate, epoxy and phenol resins, polyacrylates, polyesters, plastics and coatings, and also as a colourless colour developer (Ash & Ash, 1995; Sandell *et al.*, 1987; Okada, 1996). During the condensation, various by-products, such as BPA isomers, are formed, and these are contaminants of the desired product, *viz.* bisphenol-A. The by-product forming in the largest quantities (about 80% of all contaminants) is one of the BPA isomers, namely the title compound, (I) (also referred to as *o,p*-BPA; Hetper, 1991).



Recently, many producers of bisphenol A have undertaken studies concerning the isomerization of this by-product to *p,p*-BPA in the presence of strongly acid cation exchangers modified by compounds containing amino and sulfhydryl groups (Li, 1989; Takahashi & Takegami, 1993; Furumoto *et al.*, 1993; Kawamura *et al.*, 1994; Tasset & Wehmeyer, 1997; Heydenreich *et al.*, 2001; Sakatani *et al.*, 1996). The crystal structure of *p,p*-BPA has been known for 20 years (Belskii *et al.*, 1983), yet no structural data have been available for *o,p*-BPA, nor for compounds containing the 2,4'-isopropylidenediphenol skeleton, until now. The structural differences

between (I) and *p,p*-BPA are derived by comparison with the recently redetermined structure of *p,p*-BPA (Okada, 1996), with the same atom-numbering scheme used here.

The molecular structure of (I) is shown in Fig. 1. The two phenyl rings, C1–C6 and C11–C16, attached to atom C8, are planar, both with average out-of-plane deviations of 0.002 (2) Å. Methyl atoms C9 and C10 are nearly coplanar with these rings, with deviations from the ring planes of –0.060 (2) and –0.128 (2) Å, respectively. Similarly, the hydroxyl atoms O7 and O17 deviate from the ring planes by only –0.032 (1) and 0.000 (1) Å, respectively. The C1–C6 and C11–C16 ring planes are inclined at 84.81 (9)° to one another. This angle is in close agreement with the values of 86.9 (2), 83.6 (2) and 79.7 (2)° observed in the three independent molecules of *p,p*-BPA, as well as with the corresponding interplanar angles observed in most of the similar structures retrieved from the Cambridge Structural Database (CSD, Version 5.25 and updates; Allen, 2002). The CSD contains the results for eight different structures with the 4,4'-isopropylidenediphenol skeleton [CSD refcodes GEHJAE (Toda *et al.*, 1988), RAWDAU (Coupar *et al.*, 1997), RAWBOG (Ferguson *et al.*, 1997), SIXDOS and SIXDUY (Goldberg *et al.*, 1991), TIJVIR and TIJVEN (Eriksson & Eriksson, 2001) and UHUNAM (Takahashi *et al.*, 2003)], which have interplanar angles in the range 80–90°, and only two with by far the smallest interplanar angles of 63.9 (BIDJED; Wang *et al.*, 1982) and 64° (FATLER01; Eriksson & Eriksson, 2001). The bond lengths and valence angles in (I) are in similar ranges to those observed in *p,p*-BPA and the other above-mentioned structures. The only important difference between *o,p*-BPA and its *p,p*-isomer is the presence of one weak intramolecular hydrogen bond between methyl atom C10 and the *ortho*-substituted hydroxyl atom O7 (Table 1).

Given the close similarity of the molecular structures of the two BPA isomers, a reasonable conjecture would be that they might have rather similar crystal structures. The present investigation shows that this is not the case with respect to the packing of the molecules. Compound (I) crystallizes with four molecules in the unit cell (Fig. 2), whereas the unit cell of *p,p*-BPA [*P*2₁/*n*, *a* = 18.004 (8), *b* = 18.997 (8) and *c* = 11.235 (2) Å, and β = 100.86 (3)°], with a volume three times larger, contains 12 molecules, *i.e.* the latter contains three crystallographically independent molecules per asymmetric unit.

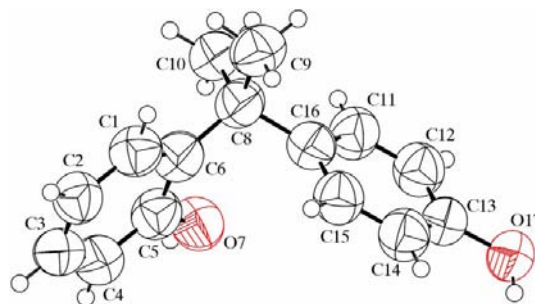


Figure 1

A view of the molecule of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

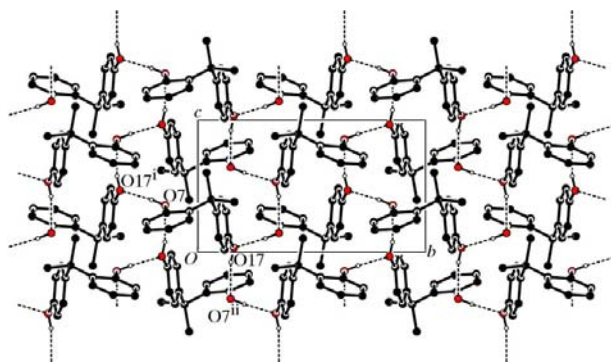


Figure 2
The unit-cell contents of (I), showing one set of intermolecular hydrogen bonds as dashed lines. All C-bound H atoms have been omitted for clarity. Symmetry codes are as given in Table 1.

The molecules of (I) are linked *via* two hydrogen bonds (Table 1), which form infinite zigzag chains running along the *c* axis. The shortest intermolecular O...O contact distance in (I) [2.798 (2) Å] is somewhat longer than the shortest intermolecular O...O contact distance in *p,p*-BPA [2.751 (9) Å] and is similar to the corresponding shortest intermolecular O...O contact distances in other similar structures (Eriksson & Eriksson, 2001; Goldberg *et al.*, 1991; Takahashi *et al.*, 2003).

Experimental

The sample of *o,p*-BPA (purity 98%) was obtained from the Institute of Heavy Organic Synthesis (Kedzierzyn-Kozle, Poland). Crystals suitable for X-ray diffraction were crystallized from ethanol by slow evaporation of the solvent at a constant temperature of 293 K.

Crystal data

$C_{15}H_{16}O_2$	$D_x = 1.238 \text{ Mg m}^{-3}$
$M_r = 228.28$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 20 reflections
$a = 13.621 (3) \text{ \AA}$	$\theta = 8\text{--}15^\circ$
$b = 12.461 (2) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 7.2320 (10) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 93.62 (3)^\circ$	Plate, colourless
$V = 1225.0 (4) \text{ \AA}^3$	$0.50 \times 0.35 \times 0.04 \text{ mm}$
$Z = 4$	

Data collection

DARCH-1 diffractometer	$R_{\text{int}} = 0.006$
$\omega/2\theta$ scans	$\theta_{\text{max}} = 27.4^\circ$
Absorption correction: refined on ΔF (DIFABS; Walker & Stuart, 1983)	$h = -17 \rightarrow 17$
$T_{\text{min}} = 0.966$, $T_{\text{max}} = 0.996$	$k = -16 \rightarrow 16$
5620 measured reflections	$l = -9 \rightarrow 9$
2810 independent reflections	3 standard reflections
1589 reflections with $I > 2\sigma(I)$	every 100 reflections
	intensity decay: 2.2%

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2]$
$wR(F^2) = 0.136$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.14$	$(\Delta/\sigma)_{\text{max}} = 0.027$
2810 reflections	$\Delta\rho_{\text{max}} = 0.08 \text{ e \AA}^{-3}$
158 parameters	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$

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

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$O7\text{--}H7\cdots O17^i$	0.82	2.00	2.798 (2)	163
$O17\text{--}H17\cdots O7^{ii}$	0.82	2.18	2.930 (2)	152
$C10\text{--}H10C\cdots O7$	0.96	2.51	3.100 (2)	120

Symmetry codes: (i) $-x, y - \frac{1}{2}, \frac{1}{2} - z$; (ii) $-x, -y, -z$.

All H atoms were refined in geometrically idealized positions, with C—H distances in the range 0.93–0.96 Å and O—H distances of 0.82 Å, and with $U_{\text{iso}}(\text{H}) = 1.5$ (for methyl and hydroxyl) or 1.2 times $U_{\text{eq}}(\text{C}, \text{O})$.

Data collection: DARCH software; cell refinement: DARCH software; data reduction: DARCH software; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2000); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GA1076). Services for accessing these data are described at the back of the journal.

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