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2,2′-Isopropylidenediphenol

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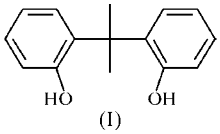
The planar benzene rings in the title compound, $C_{15}H_{16}O_2$, are inclined at an angle of 82.61 (9)° to one another. There are two intramolecular hydrogen bonds of types $O—H\cdots\pi$ and $C—H\cdots O$. The molecules are linked by strong $O—H\cdots O$ hydrogen bonds into a one-dimensional network, which is compared with that of related compounds.

Comment

The present report is a continuation of our structural studies of compounds formed, as reaction by-products, during the industrial production of 4,4′-isopropylidenediphenol (commonly referred to as bisphenol A, BPA or *p,p*-BPA) by the condensation of phenol with acetone in the presence of an acid catalyst. Examples of such by-products are the isomer 2,4′-isopropylidenediphenol (*o,p*-BPA), the title compound 2,2′-isopropylidenediphenol [(I), *o,o*-BPA], and trisphenol, polyphenols and 2,2,4-trimethyl-4-(4-hydroxyphenyl)chroman (the so-called Dianin compound) (Kiedik *et al.*, 1993). In a previous paper, we reported the structure of *o,p*-BPA [Cambridge Structural Database (Allen, 2002) refcode GALCAY (Rozycka-Sokolowska *et al.*, 2005)]. We now compare (I) with the structures of *p,p*-BPA (CEGYOC02; Okada, 1996), *o,p*-BPA and compounds containing the 2,2′-isopropylidenediphenol skeleton, *i.e.* 2,2′-isopropylidenebis(4-chloro-6-nitrophenol) (IPYCNP; Hay & Mackay, 1979) and 2,2-bis(2-hydroxy-5-methyl-3-*tert*-butylphenyl)propane (XMBPPR; Hardy & MacNicol, 1976).



(I)

As in the case of the *p,p* and *o,p* isomers of BPA and the other above-mentioned structures, the molecule of (I) contains two planar benzene rings, C1–C6 and C11–C16, attached to atom C8 (Fig. 1); the largest deviations from planarity are −0.009 (2) and −0.005 (2) Å for atoms C5 and C15, respectively. The dihedral angle between the planes formed by these rings is 82.61 (9)°. This angle is in close agreement with those found for the other isopropylidenediphenol isomers [84.81° for *o,p*-BPA, and 86.9 (2), 83.6 (2) and 79.7 (2)° for the three independent molecules of *p,p*-BPA], and with the values of 82.27 and 78.07° observed in XMBPPR and IPYCNP, respectively. Hydroxy atoms O7 and O17 are nearly coplanar with the C1–C6 and C11–C16 rings, with deviations from the ring planes of −0.034 (1) and 0.044 (1) Å, respectively; methyl atom C9 lies 0.161 (2) Å above the plane of the C1–C6 ring and atom C10 lies 0.154 (2) Å below the plane of the C11–C16 ring. The bond lengths and valence angles in (I) are within the ranges observed in the *p,p* and *o,p* isomers, and in the other compounds containing the 2,2′-isopropylidenediphenol skeleton mentioned above.

There are two weak intramolecular hydrogen-bonding contacts (Table 1 and Fig. 1); the first involves hydroxy atom H17 interacting with the C1–C6 ring in a classical intramolecular $O—H\cdots\pi$ hydrogen bond (Desiraju & Steiner, 1999). The $H\cdots C$ distances between atom H17 and the nearest C atoms belonging to the C1–C6 ring are 2.43 (2) (for $H17\cdots C1$) and 2.19 (2) Å (for $H17\cdots C6$), and they are similar to the corresponding $H\cdots C$ distances found for XMBPPR, 2,6-diphenylphenol (DPPHOL; Nakatsu *et al.*, 1978) and bis(2-hydroxy-3-*tert*-butylphenyl)methane (NISQUB; Böhmer *et al.*, 1996). The second $C—H\cdots O$ interaction, between the methyl group (atom C10) and hydroxy atom O7 (Fig. 1), generates an *S*(6) graph-set motif (Bernstein *et al.*, 1995). The presence of this latter weak intramolecular hydrogen bond is a common characteristic of the *o,p* and *o,o* isomers of isopropylidenediphenol and is an important difference between these isomers and the *p,p* isomer. Analysis of geometrical parameters of the intramolecular $C—H\cdots O$ hydrogen bonds presented here and in *o,p*-BPA shows a close similarity; the $H\cdots O$ and $C\cdots O$ distances and the $C—H\cdots O$ angle in (I) are similar to those found for the *o,p* isomer [$H\cdots O$ = 2.51 Å, $C\cdots O$ = 3.100 (2) Å and $C—H\cdots O$ = 120° (GALCAY; Rozycka-Sokolowska *et al.*, 2005)].

The packing structure of (I) involves one strong intermolecular hydrogen bond (Steiner, 2002) (Table 1), which links adjacent molecules into a chain, running parallel to the

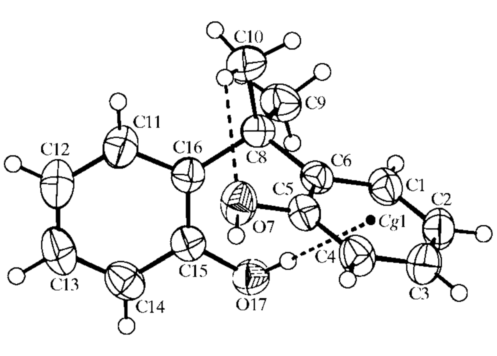


Figure 1
The constituent molecule of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines depict the intramolecular hydrogen bonds. H atoms are drawn as spheres of arbitrary radii. The centroid (*Cg*1) of the C1–C6 ring is denoted by a small black circle.

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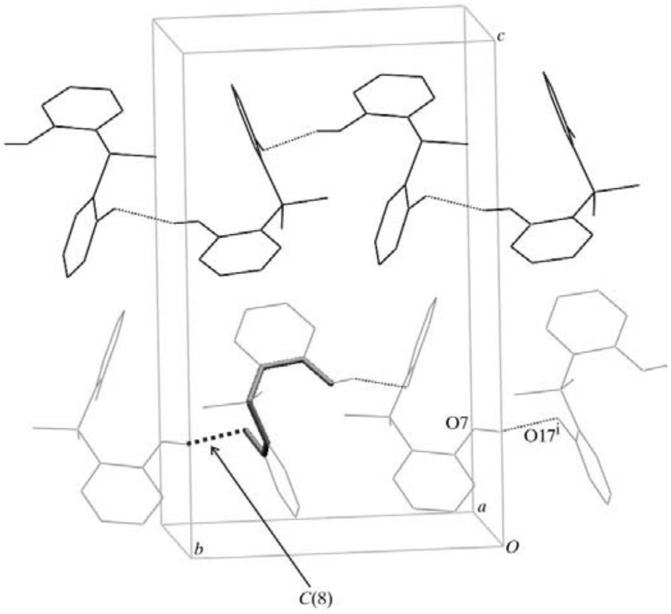

Figure 2
Part of the crystal structure of (I), showing two $C(8)$ chains of molecules lying in domains $0.05 < c < 0.45$ (molecules drawn with grey lines) and $0.55 < c < 0.95$ (molecules drawn with black lines) [symmetry code: (i) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$]. H atoms not involved in hydrogen bonding have been omitted for clarity.

[010] direction, with a graph-set motif of $C(8)$ (Bernstein *et al.*, 1995) (Fig. 2). The two chains passing through each unit cell are antiparallel with no direction-specific interactions between adjacent chains.

A similar one-dimensional hydrogen-bond network is found in 2,2′-diphenol (NUTSUQ; Byrne *et al.*, 1998) and its derivatives, such as 2,2′-dihydroxy-5,5′-diallylbiphenyl (CIPXII; Wang *et al.*, 1983), 5,5′-di-*tert*-butylbiphenyl-2,2′-diol and 5,5′-dimethylbiphenyl-2,2′-diol (MEBMIP and MEBMOV, respectively; Bocelli *et al.*, 1999). By contrast, a totally different molecular arrangement is found in the *o,p* and *p,p* isomers of (I). The molecules of *o,p*-BPA are connected by two independent intermolecular O—H···O hydrogen bonds into a two-dimensional sheet of six-membered rings, which is parallel to (100), while the molecules of *p,p*-BPA are connected by a combination of six O—H···O and one C—H···O hydrogen bonds into a three-dimensional network built from many four- and six-membered rings. In summary, significant packing changes occur through hydrogen-bond networks found for these compounds, from three-dimensional for the *p,p* isomer, through two-dimensional for the *o,p* isomer, to a one-dimensional network here for the *o,o* isomer, all related to the moving of one (in *o,p*-BPA) or two (in *o,o*-BPA) hydroxy substituents from the *para* to the *ortho* position.

Experimental

The sample of *o,o*-BPA 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

$C_{15}H_{16}O_2$
$M_r = 228.28$
Orthorhombic, $P2_12_12_1$
$a = 7.032$ (1) Å
$b = 10.419$ (2) Å
$c = 17.017$ (3) Å
$V = 1246.8$ (4) Å^3
$Z = 4$
$D_x = 1.216$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 35 reflections
$\theta = 6$–$20°$
$\mu = 0.63$ mm^{-1}
$T = 288$ (1) K
Block, colourless
$0.23 \times 0.21 \times 0.11$ mm

Data collection

Kuma KM-4 diffractometer
ω–2θ scans
8248 measured reflections
1343 independent reflections
1163 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\rm max} = 68.1°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 12$
$l = -14 \rightarrow 20$
3 standard reflections every 100 reflections intensity decay: 1.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.071$
$S = 1.03$
1343 reflections
165 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 0.0854P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.15$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.09$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0042 (6)

Table 1
Hydrogen bonding geometry (Å, °).

*Cg*1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7···O17^{i}	0.88 (3)	2.00 (3)	2.843 (2)	160 (2)
C10—H10*A*···O7	0.96	2.45	3.031 (2)	119
O17—H17···*Cg*1	0.86 (2)	2.68	3.491	159

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

All C-bound H atoms were refined in geometrically idealized positions, with C—H distances of 0.93 (aromatic) and 0.96 Å (methyl groups), and with $U_{\rm iso}$(H) values of 1.2 (aromatic) or 1.5 (CH_3) times $U_{\rm eq}$(C). The H atoms of hydroxy groups were located in difference maps and refined isotropically. Friedel equivalent data were merged using MERG4 in *SHELXL97* (Sheldrick, 1997), according to the standard procedure for X-ray measurements of chemical compounds without atoms heavier than Si.

Data collection: *KM4B8* (Gałdecki *et al.*, 1996); cell refinement: *KM4B8*; data reduction: *KM4B8*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2000) and *MERCURY* (Version 1.4; Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GA1119). Services for accessing these data are described at the back of the journal.

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