

2,6-Di-*tert*-butyl-4-(hydroxymethyl)phenolGuo-Yi Bai,^{a*} Jim Simpson,^b
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Key indicators

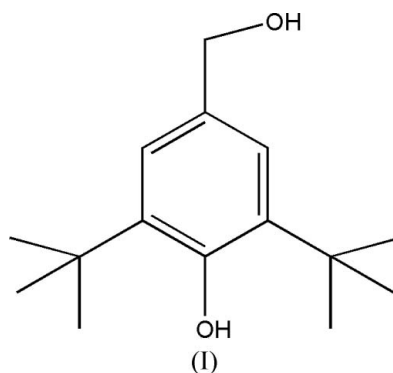
Single-crystal X-ray study
 $T = 294\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
Disorder in main residue
 R factor = 0.064
 wR factor = 0.201
Data-to-parameter ratio = 8.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The molecule of the title compound, $\text{C}_{15}\text{H}_{24}\text{O}_2$, lies across a mirror plane with the two *tert*-butyl substituents flanking the phenolic OH group in this hindered phenol. In the crystal structure, $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds between the benzylic OH group and the phenolic O atom link the molecules into chains.

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Comment

The title compound (I) belongs to a class of compounds known as hindered phenols that are widely used as anti-oxidants (Silin *et al.*, 1999). We report here the preparation and crystal structure of (I) (Fig. 1). The molecule lies across a mirror plane with the phenolic OH group, atom C1, C4, and the benzylic atom C9 atom on the mirror plane. Atoms O2 and H2 of the benzylic OH and the H atoms on C9 are disordered about the mirror plane. Bond distances and angles within the molecule are normal (Allen *et al.*, 1987) and similar to those found in related compounds (Xin *et al.*, 2006; Zeng *et al.*, 2005; Bukharov *et al.*, 2001; Imura *et al.*, 1983). A crystal structure solved in the same space group as (I) with very similar unit-cell parameters (18.580, 6.150, 6.100 Å, 90, 90, 90°; no s.u.'s given; Takagi *et al.*, 1992) was reported as being 2,6-di-*tert*-butyl-4-formylphenol, but there are no three-dimensional coordinates available, nor are geometric parameters published for comparison with the title compound. In (I), the aryl ring and the non-H substituents lie in a plane, the maximum deviation from the plane though atoms C1–C5, C9, O1 being 0.004 (4) Å for C1. Atom C8 atom of the *tert*-butyl substituent lies only 0.025 (7) Å from this plane.



In the crystal structure, molecules are linked by an intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond (Fig. 2), forming approximately orthogonal sets of molecular chains that alternate both in and perpendicular to the *ac* plane. The packing is further stabilized by weak $\text{C}-\text{H}\cdots\text{O}$ interactions (Table 2) that augment the classical hydrogen bond and link the molecular chains.

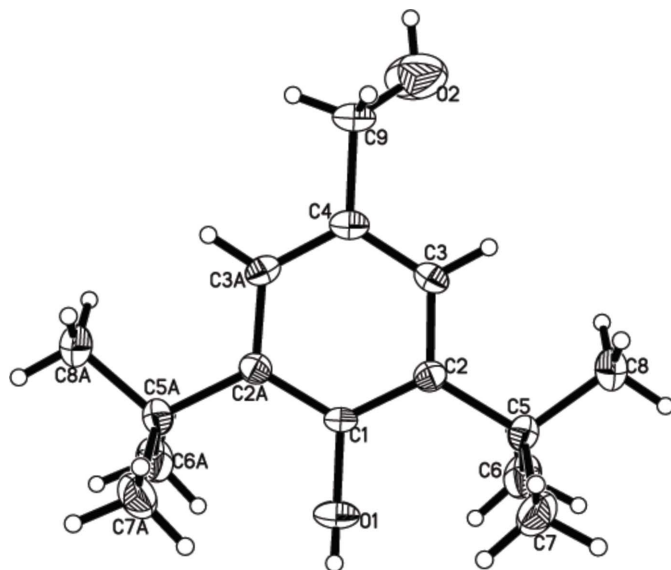


Figure 1
The molecular structure of (I). The second components of the disordered hydroxyl group and H atoms are omitted for clarity.

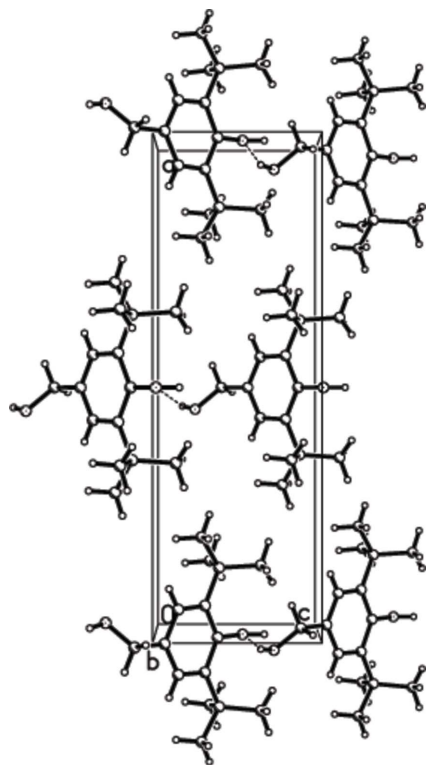


Figure 2
A partial packing diagram for (I). The dashed lines indicate intermolecular hydrogen bonds. The second components of the disordered hydroxyl group and H atoms are omitted for clarity.

Experimental

The title compound was obtained by the reduction of 3,5-di-*tert*-butyl-4-hydroxybenzaldehyde (2.36 g, 10 mmol) with sodium borohydride (0.72, 20 mmol) in dry ethanol (20 ml) (yield 80.4%, m.p.

412–413 K). Crystals for X-ray diffraction were grown from a benzene solution at room temperature.

Crystal data

$C_{15}H_{24}O_2$ $Z = 2$
 $M_r = 236.34$ $D_x = 1.059 \text{ Mg m}^{-3}$
 Orthorhombic, $Pmn2_1$ Mo $K\alpha$ radiation
 $a = 18.901 (5) \text{ \AA}$ $\mu = 0.07 \text{ mm}^{-1}$
 $b = 6.2580 (14) \text{ \AA}$ $T = 294 (2) \text{ K}$
 $c = 6.2670 (19) \text{ \AA}$ Block, colourless
 $V = 741.3 (3) \text{ \AA}^3$ $0.32 \times 0.28 \times 0.24 \text{ mm}$

Data collection

Bruker SMART CCD area-detector 3466 measured reflections
 diffractometer 740 independent reflections
 φ and ω scans 685 reflections with $I > 2\sigma(I)$
 Absorption correction: multi-scan $R_{\text{int}} = 0.032$
 (SADABS; Bruker, 1997) $\theta_{\text{max}} = 25.0^\circ$
 $T_{\text{min}} = 0.979$, $T_{\text{max}} = 0.984$

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.1499P)^2 + 0.1064P]$
 $R[F^2 > 2\sigma(F^2)] = 0.064$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.201$ $(\Delta/\sigma)_{\text{max}} = 0.001$
 $S = 1.12$ $\Delta\rho_{\text{max}} = 0.49 \text{ e \AA}^{-3}$
 740 reflections $\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
 92 parameters
 H-atom parameters constrained

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O2-H2A \cdots O1^i$	0.85	1.90	2.707 (10)	159
$C6-H6B \cdots O2^{ii}$	0.96	2.67	3.571 (10)	157
$C7-H7B \cdots O2^{iii}$	0.96	2.63	3.457 (11)	145

Symmetry codes: (i) $x, y + 1, z - 1$; (ii) $x, y - 1, z + 1$; (iii) $x, y, z + 1$.

In the absence of significant anomalous dispersion effects, Friedel pairs were merged. The phenolic H atom H1, the O2 hydroxyl group and two H atoms on C9 are disordered over the mirror plane and were refined with site occupancies fixed at 0.5. The H atoms of the disordered OH and CH_2 groups were located in a difference Fourier map and refined as riding on their carrier atoms. Other H atoms were placed in calculated positions and treated as riding with $C-H = 0.93 \text{ \AA}$, $U_{\text{iso}} = 1.2U_{\text{eq}}(C)$ for aromatic H and $C-H = 0.96 \text{ \AA}$, $U_{\text{iso}} = 1.5U_{\text{eq}}(C)$ for methyl H atoms.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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