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New polymorph of 2,6-dimethylphenol

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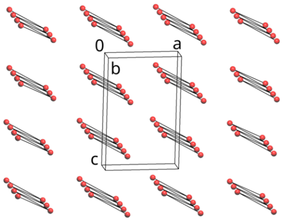
The racemic monoclinic polymorph of the title compound, $C_8H_{10}O$, is known from the literature [Antona *et al.* (1973). *Acta Cryst.* B**29**, 1372–1376] and has been redetermined here. Additionally, a new enantiopure orthorhombic polymorph is reported. The strongest intermolecular interactions are within one-dimensional hydrogen-bonded chains which are very similar in the two polymorphs. On the other hand, the packing of the chains in the crystal differs significantly between the two forms.



1. Chemical context

Phenolic compounds are important antioxidants which occur in biological systems and are present in beverages such as coffee and tea. They are also artificially added to industrial processes to prevent oxidation. Thereby the phenolic hydroxy group is oxidized to a peroxide and steric strain of substituents at the ring strongly influence this reaction (Drew *et al.*, 1990). In the medical world, the compound 2,6-diisopropylphenol is a relevant drug which is distributed under the name Propofol.

In crystal engineering, phenols belong to the category of bulky alcohols (Brock & Duncan, 1994). Here, the steric demand of the ring substituents influences the hydrogen-bonding pattern. If the hydroxy group is the only functional group, it can act both as hydrogen-bond donor and as hydrogen-bond acceptor. For example, unsubstituted phenol in its monoclinic ambient-pressure polymorph forms one-dimensional hydrogen-bonded chains (Zavodnik *et al.*, 1987). The three independent molecules which constitute the chain are related only by pure translations. The monoclinic high-pressure variant of 2-methylphenol again forms one-dimensional hydrogen-bonded chains, but in this structure there is only one independent molecule and the fundamental symmetry operation in the chain is a 2_1 screw axis along the *b* direction (Oswald & Crichton, 2009). The corresponding length of the *b* axis is 4.7006 (3) Å. In the crystal structure of 2,6-diisopropylphenol, there are hydrogen-bonded tetramers (Bacchi *et al.*, 2016) and in 2,6-di-*tert*-butylphenol, there are no hydrogen bonds (Lutz & Spek, 2005).

2. Structural commentary

The crystal structure of the title compound was reported in the literature as monoclinic with the space group $P2_1/c$. Preliminary investigations and unit-cell parameters were reported by Meuthen & von Stackelberg (1960). A full structure determination by Antona *et al.* (1973) was based on intensities from film methods [Cambridge Structural Database (CSD; Groom *et al.*, 2016) refcode DMEPOL10]. In order to improve the quality of the results, we re-investigated this crystal

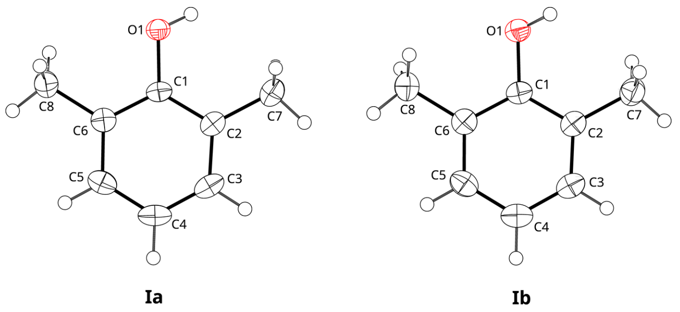
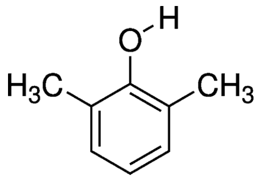


Figure 1
The molecular structures of (Ia) (monoclinic) and (Ib) (orthorhombic). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn with arbitrary radii.

structure with modern equipment and the results are presented here [structure (Ia)]. During our studies, we additionally found a new orthorhombic polymorph with the space group $P2_12_12_1$ [structure (Ib)]. This structure will also be presented and both polymorphs will be compared.



The molecular structures of the monoclinic (Ia) and orthorhombic (Ib) polymorphs are very similar and differ only in the conformations of the methyl groups (Fig. 1). There are no significant differences in the bond lengths and angles between the two structures (Tables 1 and 2). The molecules are essentially planar, with a maximum deviation from the plane of 0.0330 (9) Å for atom O1 in (Ia) and 0.0158 (17) Å for atom C1 in (Ib). Consequently, the non-H atoms of the molecule have approximate C_{2v} symmetry, with an r.m.s. deviation of 0.0754 Å for (Ia) and 0.0725 Å for (Ib).

Table 1
Comparison of bond lengths (Å) in (Ia) and (Ib).

	(Ia)	(Ib)	Δ	Δ/σ
O1—C1	1.3862 (16)	1.3913 (19)	−0.0051 (25)	−2.04
C1—C6	1.393 (2)	1.392 (2)	0.0010 (28)	0.36
C1—C2	1.3958 (19)	1.398 (2)	−0.0022 (28)	−0.79
C2—C3	1.3892 (19)	1.389 (2)	0.0002 (28)	0.07
C2—C7	1.496 (2)	1.503 (3)	−0.007 (4)	−1.75
C3—C4	1.378 (2)	1.380 (3)	−0.002 (4)	−0.50
C4—C5	1.382 (2)	1.385 (3)	−0.003 (4)	−0.75
C5—C6	1.389 (2)	1.387 (2)	0.0020 (28)	0.71
C6—C8	1.5068 (19)	1.509 (3)	−0.002 (4)	−0.50

Table 2
Comparison of bond angles (°) in (Ia) and (Ib).

	(Ia)	(Ib)	Δ	Δ/σ
O1—C1—C6	116.06 (12)	116.36 (15)	−0.30 (19)	−1.58
O1—C1—C2	121.67 (13)	121.28 (16)	0.39 (21)	1.85
C6—C1—C2	122.24 (12)	122.32 (16)	−0.08 (20)	−0.40
C3—C2—C1	117.39 (14)	117.38 (17)	0.01 (22)	0.05
C3—C2—C7	121.12 (13)	120.93 (17)	0.19 (21)	0.90
C1—C2—C7	121.50 (12)	121.69 (16)	−0.19 (20)	−0.95
C4—C3—C2	121.72 (14)	121.58 (18)	0.14 (23)	0.61
C3—C4—C5	119.59 (14)	119.64 (18)	−0.05 (23)	−0.22
C4—C5—C6	121.03 (15)	121.01 (19)	0.02 (24)	0.08
C5—C6—C1	118.03 (13)	118.05 (16)	−0.02 (21)	−0.10
C5—C6—C8	120.96 (14)	121.06 (17)	−0.10 (22)	−0.45
C1—C6—C8	121.01 (12)	120.88 (16)	0.13 (20)	0.65

3. Supramolecular features

The hydrogen-bonding patterns in (Ia) and (Ib) are very similar (Fig. 2, and Tables 3 and 4). The molecules form one-dimensional chains, in (Ia) along the *b* axis and in (Ib) along the *a* axis. In both cases, the symmetry operation relating the molecules within one chain is a 2_1 screw axis. In (Ia), the unit-cell length of the *b* axis is 4.45179 (19) Å and in (Ib) the *a* axis is 4.3981 (4) Å. By the screw symmetry, each individual chain is helically chiral. In centrosymmetric (Ia), the overall structure is racemic, and in (Ib) the overall structure is enantiopure. The absolute structure of (Ib) could not be determined reliably from anomalous scattering. The one-dimensional chains

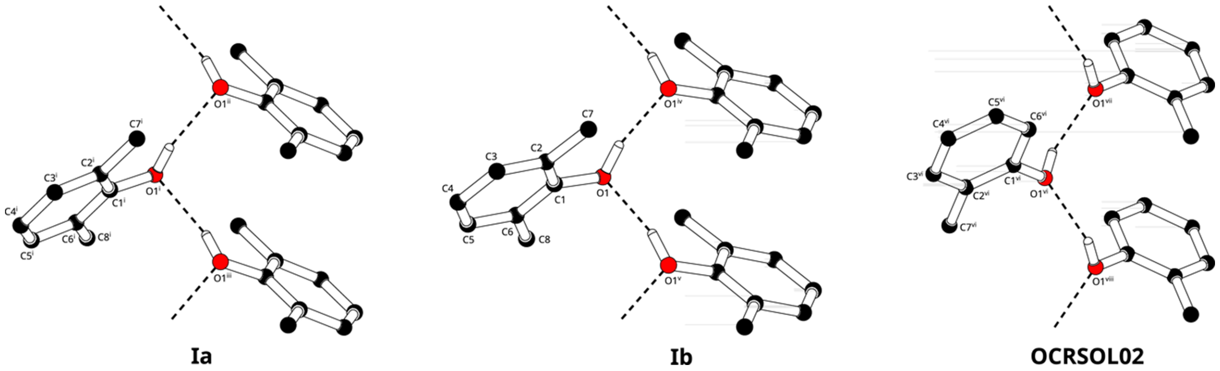


Figure 2
Hydrogen-bonded one-dimensional chains. C—H hydrogens are omitted for clarity. For (Ia), the *b* axis is oriented verically in the plane of the drawing. [Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1, -y+\frac{1}{2}, z+\frac{1}{2}$; (iii) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.] For (Ib), the *a* axis is oriented verically in the plane of the drawing. [Symmetry codes: (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$; (v) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+2$.] For 2-methylphenol (CSD refcode OCRSOL02; Oswald & Crichton, 2009), the *b* axis is oriented verically in the plane of the drawing. [Symmetry codes: (vi) $-x+1, -y+1, -z+1$; (vii) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$; (viii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.]

Table 3
Hydrogen-bond geometry (Å, °) for (Ia).

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
$O1—H1\cdots O1^{i}$	0.840 (19)	2.032 (18)	2.8087 (12)	153.4 (15)

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

Table 4
Hydrogen-bond geometry (Å, °) for (Ib).

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
$O1—H1\cdots O1^{i}$	0.90 (3)	1.89 (3)	2.7470 (14)	158 (2)

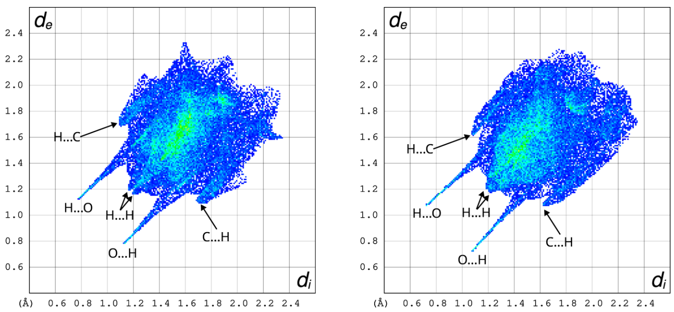
Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+2$.

are comparable with racemic 2-methylphenol (Oswald & Crichton, 2009; CSD refcode OCRSOL02). While the O—H···O geometry in the three structures is similar, the arrangement of the molecular planes differs slightly. In (Ia), the molecular plane has an angle of 53.11 (3)° with the *b* axis, in (Ib) there is an angle of 55.58 (4)° with the *a* axis and in 2-methylphenol there is an angle of 47.20 (11)° with the *b* axis.

As a consequence of the hydrogen-bonding scheme, the C—C—O—H torsion angles are similar: 20.2 (13)° in racemic (Ia) and −30.0 (18)° in (Ib). This is in contrast to 2,6-di-*tert*-butylphenol (Lutz & Spek, 2005) which does not form hydrogen bonds and where the hydroxy group is in the molecular plane.

In addition to the hydrogen bonding, there are weak π–π stacking interactions within the chains, *i.e.* along the *b* direction in (Ia) and along the *a* direction in (Ib). The corresponding symmetry operations are pure translations (Table 5). Consequently, the involved rings are exactly parallel, but because the rings are tilted with respect to the crystallographic axes, respectively, the ring slippage is rather large.

The geometrical analysis of intermolecular interactions is confirmed by the calculation of Hirshfeld surface fingerprint plots (McKinnon *et al.*, 2004) for (Ia) and (Ib), which show a high similarity between the two polymorphs (Fig. 3). This similarity is a strong indication that all major intermolecular bonds are within the hydrogen-bonded chains. Enrichment ratios (Jelsch *et al.*, 2014) derived from the fingerprint plots (Tables 6 and 7) highlight the propensity for H···O and C···C interactions, *i.e.* hydrogen bonds and π–π stacking.



Ia **Ib**

Figure 3
Hirshfeld surface fingerprint plots (McKinnon *et al.*, 2004) for (Ia) and (Ib) prepared with *CrystalExplorer* (Version 21.5; Spackman *et al.*, 2021).

Table 5
Weak π–π stacking in (Ia) and (Ib).

Cg stands for center of gravity.

Structure	Ring···ring	Perpendicular ring–ring distance (Å)	$Cg\cdots Cg$ distance (Å)	Slippage (Å)
(Ia)	$C1–C6\cdots C1–C6^{i}$	3.5387 (6)	4.4518 (9)	2.701
(Ib)	$C1–C6\cdots C1–C6^{ii}$	3.6085 (8)	4.3981 (12)	2.514

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

Table 6
Enrichment ratios for (Ia) calculated by the approach of Jelsch *et al.* (2014) from the Hirshfeld surface fingerprint plot.

	H	C	O
H	1.00	–	–
C	0.94	1.78	–
O	1.22	–	–

Table 7
Enrichment ratios for (Ib) calculated by the approach of Jelsch *et al.* (2014) from the Hirshfeld surface fingerprint plot.

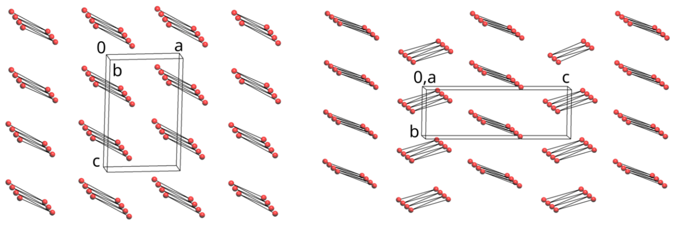
	H	C	O
H	1.00	–	–
C	0.91	1.95	–
O	1.21	–	–

While the geometry within the hydrogen-bonded chains in (Ia) and (Ib) is very similar, the packing of the chains is significantly different (Fig. 4). The inversion centres between the chains in (Ia) result in the coplanarity of the rings in adjacent chains. The chains in (Ib) are related to each other by 2_1 screw axes, resulting in a dihedral angle of 50.70° between the planes of the rings in adjacent chains.

Despite the different packing of the chains, the crystal density in (Ia) and (Ib) is very similar with values of 1.1754 (1) and 1.1819 (1) g cm^{3}, respectively. The corresponding packing indices (Kitajgorodskij, 1973) of 68.4% for (Ia) and 69.0% for (Ib) are consistent with this. Based on this information, it cannot be decided which of the two polymorphs is more stable.

4. Synthesis and crystallization

Commercial 2,6-dimethylphenol (Sigma–Aldrich) was used as starting material. Crystals of (Ia) were obtained by slow



Ia **Ib**

Figure 4
Simplified structures of (Ia) and (Ib). Red spheres are the simplified individual molecules of 2,6-dimethylphenol and the connecting lines are the O—H···O hydrogen bonds. Simplification and plot preparation was done with *ToposPro* (Blatov *et al.*, 2014).

Table 8
Experimental details.

For both structures: $C_8H_{10}O$, M_r = 122.16, Z = 4. Experiments were carried out at 150 K with Mo $K\alpha$ radiation using a Bruker Kappa APEXII area-detector diffractometer. Absorption was corrected for by multi-scan methods (*SADABS2016*; Krause *et al.*, 2015). Refinement was on 88 parameters. H atoms were treated by a mixture of independent and constrained refinement.

	(Ia)	(Ib)
Crystal data		
Crystal system, space group	Monoclinic, $P2_1/c$	Orthorhombic, $P2_12_12_1$
a, b, c (Å)	10.0160 (5), 4.45179 (19), 15.4874 (7)	4.3981 (4), 7.2646 (4), 21.4884 (12)
α, β, γ (°)	90, 91.533 (3), 90	90, 90, 90
V (Å^3)	690.32 (6)	686.56 (8)
μ (mm^{-1})	0.08	0.08
Crystal size (mm)	0.27 × 0.10 × 0.05	0.29 × 0.13 × 0.08
Data collection		
$T_{\min}$, $T_{\max}$	0.635, 0.746	0.572, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12932, 1585, 1058	9552, 1583, 1372
R_{int}	0.054	0.030
(sin $\theta/\lambda)_{\max}$ (Å^{-1})	0.650	0.650
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.106, 1.04	0.038, 0.089, 1.06
No. of reflections	1585	1583
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.19, −0.16	0.12, −0.15
Absolute structure	–	Flack x determined using 493 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	–	0.2 (6)

Computer programs: *APEX3* (Bruker, 2012), *PEAKREF* (Schreurs, 2016), *Eval15* (Schreurs *et al.*, 2010), *SADABS2016* (Krause *et al.*, 2015), *SHELXS* (Sheldrick, 2008), *SHELXL2019* (Sheldrick, 2015), *PLATON* (Spek, 2020), *CrystalExplorer* (Spackman *et al.*, 2021) and *TopoPro* (Blatov *et al.*, 2014).

evaporation from a solution in hexane. Crystals of (Ib) were obtained by slow evaporation from a solution in ethanol. Note that the hexane solution gave crystals of both forms. Both crystal forms are very brittle and difficult to cut.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 8. The intensity integration of (Ia) involved a large isotropic mosaicity of 1.3° for the prediction of the reflection profiles. For (Ib), an isotropic mosaicity of 1.5° plus an anisotropic mosaicity of 0.45° about *hkl*=(0,0,1) was involved.

In the refinements of (Ia) and (Ib), O—H hydrogens were refined freely with isotropic displacement parameters and C—H hydrogens were refined with a riding model.

Acknowledgements

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New polymorph of 2,6-dimethylphenol

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Computing details

2,6-Dimethylphenol (Ia)

Crystal data

$C_8H_{10}O$
$M_r = 122.16$
Monoclinic, $P2_1/c$
$a = 10.0160$ (5) Å
$b = 4.45179$ (19) Å
$c = 15.4874$ (7) Å
$\beta = 91.533$ (3)°
$V = 690.32$ (6) Å^3
$Z = 4$
$F(000) = 264$
$D_x = 1.175$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5797 reflections
$\theta = 1.3$–27.5°
$\mu = 0.08$ mm^{-1}
$T = 150$ K
Needle, colourless
0.27 × 0.10 × 0.05 mm

Data collection

Bruker Kappa APEXII area detector diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS2016; Krause *et al.*, 2015)
$T_{min} = 0.635$, $T_{max} = 0.746$
12932 measured reflections
1585 independent reflections
1058 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.0°$
$h = -13 \rightarrow 13$
$k = -5 \rightarrow 5$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.106$
$S = 1.04$
1585 reflections
88 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.1557P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
O1	0.08542 (10)	0.5797 (2)	0.24855 (6)	0.0284 (3)
H1	0.0445 (17)	0.732 (4)	0.2661 (11)	0.048 (6)*
C1	0.18926 (13)	0.4937 (3)	0.30414 (9)	0.0245 (3)
C2	0.19468 (13)	0.5837 (3)	0.39048 (9)	0.0273 (3)
C3	0.30044 (15)	0.4779 (4)	0.44177 (9)	0.0348 (4)
H3	0.307081	0.537423	0.500640	0.042*
C4	0.39598 (15)	0.2888 (4)	0.40949 (10)	0.0390 (4)
H4	0.466787	0.217345	0.445997	0.047*
C5	0.38813 (14)	0.2039 (4)	0.32369 (10)	0.0358 (4)
H5	0.454183	0.073940	0.301499	0.043*
C6	0.28515 (14)	0.3056 (3)	0.26936 (9)	0.0289 (3)
C7	0.09068 (16)	0.7856 (4)	0.42675 (9)	0.0356 (4)
H7A	0.088815	0.975694	0.394838	0.053*
H7B	0.112039	0.824889	0.487829	0.053*
H7C	0.003074	0.688351	0.421333	0.053*
C8	0.27789 (15)	0.2164 (4)	0.17549 (9)	0.0375 (4)
H8A	0.205148	0.071901	0.166053	0.056*
H8B	0.362625	0.124388	0.159553	0.056*
H8C	0.261160	0.395016	0.139823	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0301 (6)	0.0258 (6)	0.0289 (6)	0.0026 (5)	−0.0060 (4)	−0.0013 (5)
C1	0.0239 (7)	0.0218 (7)	0.0275 (7)	−0.0058 (6)	−0.0050 (6)	0.0045 (6)
C2	0.0306 (7)	0.0251 (8)	0.0261 (7)	−0.0082 (6)	0.0000 (6)	0.0028 (6)
C3	0.0399 (8)	0.0370 (9)	0.0271 (8)	−0.0116 (7)	−0.0075 (7)	0.0049 (7)
C4	0.0306 (8)	0.0420 (10)	0.0436 (9)	−0.0031 (7)	−0.0123 (7)	0.0109 (8)
C5	0.0269 (7)	0.0347 (9)	0.0457 (9)	0.0015 (7)	−0.0019 (7)	0.0040 (7)
C6	0.0272 (7)	0.0277 (8)	0.0317 (8)	−0.0046 (6)	0.0004 (6)	0.0015 (6)
C7	0.0439 (9)	0.0356 (9)	0.0275 (8)	−0.0030 (7)	0.0017 (6)	−0.0012 (7)
C8	0.0344 (8)	0.0420 (10)	0.0363 (9)	0.0036 (7)	0.0020 (7)	−0.0072 (7)

Geometric parameters (Å, º)

O1—C1	1.3862 (16)	C5—C6	1.389 (2)
O1—H1	0.840 (19)	C5—H5	0.9500
C1—C6	1.393 (2)	C6—C8	1.5068 (19)
C1—C2	1.3958 (19)	C7—H7A	0.9800
C2—C3	1.3892 (19)	C7—H7B	0.9800
C2—C7	1.496 (2)	C7—H7C	0.9800
C3—C4	1.378 (2)	C8—H8A	0.9800
C3—H3	0.9500	C8—H8B	0.9800
C4—C5	1.382 (2)	C8—H8C	0.9800
C4—H4	0.9500		

C1—O1—H1	112.7 (11)	C5—C6—C1	118.03 (13)
O1—C1—C6	116.06 (12)	C5—C6—C8	120.96 (14)
O1—C1—C2	121.67 (13)	C1—C6—C8	121.01 (12)
C6—C1—C2	122.24 (12)	C2—C7—H7A	109.5
C3—C2—C1	117.39 (14)	C2—C7—H7B	109.5
C3—C2—C7	121.12 (13)	H7A—C7—H7B	109.5
C1—C2—C7	121.50 (12)	C2—C7—H7C	109.5
C4—C3—C2	121.72 (14)	H7A—C7—H7C	109.5
C4—C3—H3	119.1	H7B—C7—H7C	109.5
C2—C3—H3	119.1	C6—C8—H8A	109.5
C3—C4—C5	119.59 (14)	C6—C8—H8B	109.5
C3—C4—H4	120.2	H8A—C8—H8B	109.5
C5—C4—H4	120.2	C6—C8—H8C	109.5
C4—C5—C6	121.03 (15)	H8A—C8—H8C	109.5
C4—C5—H5	119.5	H8B—C8—H8C	109.5
C6—C5—H5	119.5		

O1—C1—C2—C3	177.94 (12)	C3—C4—C5—C6	−0.2 (2)
C6—C1—C2—C3	−0.1 (2)	C4—C5—C6—C1	−0.6 (2)
O1—C1—C2—C7	−1.9 (2)	C4—C5—C6—C8	179.08 (14)
C6—C1—C2—C7	−179.92 (13)	O1—C1—C6—C5	−177.45 (12)
C1—C2—C3—C4	−0.7 (2)	C2—C1—C6—C5	0.7 (2)
C7—C2—C3—C4	179.16 (14)	O1—C1—C6—C8	2.9 (2)
C2—C3—C4—C5	0.8 (2)	C2—C1—C6—C8	−178.95 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{i}	0.840 (19)	2.032 (18)	2.8087 (12)	153.4 (15)

Symmetry code: (i) −*x*, *y*+1/2, −*z*+1/2.

2,6-Dimethylphenol (Ib)

Crystal data

$C_8H_{10}O$	D_x = 1.182 Mg m^{-3}
M_r = 122.16	Mo *Kα* radiation, *λ* = 0.71073 Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 6677 reflections
a = 4.3981 (4) Å	*θ* = 1.9–27.6°
b = 7.2646 (4) Å	*μ* = 0.08 mm^{-1}
c = 21.4884 (12) Å	*T* = 150 K
V = 686.56 (8) Å^3	Needle, colourless
Z = 4	0.29 × 0.13 × 0.08 mm
F(000) = 264	

Data collection

Bruker Kappa APEXII area detector diffractometer	Absorption correction: multi-scan (SADABS2016; Krause *et al.*, 2015)
Radiation source: sealed tube	T_{min} = 0.572, T_{max} = 0.746
φ and *ω* scans	9552 measured reflections

1583 independent reflections
1372 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.030$
$\theta_{\text{max}} = 27.5°$, $\theta_{\text{min}} = 1.9°$

$h = -5 \rightarrow 5$
$k = -9 \rightarrow 9$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.089$
$S = 1.06$
1583 reflections
88 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: difference Fourier map
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 0.1305P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\text{max}} < 0.001$
$\Delta\rho_{\text{max}} = 0.12$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.15$ e Å^{-3}
Absolute structure: Flack *x* determined using 493 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: 0.2 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.0115 (3)	0.24139 (17)	0.96180 (5)	0.0332 (3)
H1	0.188 (6)	0.271 (4)	0.9805 (10)	0.056 (7)*
C1	−0.0283 (4)	0.3341 (2)	0.90574 (7)	0.0282 (4)
C2	0.0962 (4)	0.5089 (2)	0.89606 (8)	0.0305 (4)
C3	0.0425 (5)	0.5920 (3)	0.83892 (8)	0.0362 (5)
H3	0.128018	0.709627	0.830709	0.043*
C4	−0.1321 (5)	0.5079 (3)	0.79378 (9)	0.0408 (5)
H4	−0.166637	0.567537	0.755069	0.049*
C5	−0.2567 (5)	0.3362 (3)	0.80521 (8)	0.0379 (5)
H5	−0.378602	0.279108	0.774230	0.046*
C6	−0.2063 (4)	0.2462 (3)	0.86119 (8)	0.0314 (4)
C7	0.2806 (5)	0.6043 (3)	0.94534 (9)	0.0383 (5)
H7A	0.476881	0.541912	0.949973	0.058*
H7B	0.170690	0.600535	0.984991	0.058*
H7C	0.314514	0.732705	0.933190	0.058*
C8	−0.3386 (5)	0.0581 (3)	0.87339 (9)	0.0400 (5)
H8A	−0.506899	0.068676	0.903074	0.060*
H8B	−0.181070	−0.022347	0.890737	0.060*
H8C	−0.413907	0.005669	0.834295	0.060*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0344 (8)	0.0349 (6)	0.0305 (6)	−0.0030 (7)	−0.0010 (6)	0.0056 (5)
C1	0.0286 (9)	0.0295 (8)	0.0264 (8)	0.0054 (8)	0.0056 (7)	0.0014 (7)
C2	0.0301 (9)	0.0286 (8)	0.0328 (9)	0.0040 (8)	0.0060 (7)	−0.0008 (7)
C3	0.0393 (11)	0.0326 (9)	0.0367 (9)	0.0033 (9)	0.0070 (9)	0.0053 (8)
C4	0.0439 (12)	0.0461 (11)	0.0323 (9)	0.0065 (11)	0.0020 (9)	0.0080 (8)
C5	0.0378 (11)	0.0461 (11)	0.0299 (9)	0.0027 (10)	−0.0009 (8)	−0.0031 (8)
C6	0.0304 (9)	0.0317 (9)	0.0320 (9)	0.0036 (9)	0.0048 (7)	−0.0028 (7)
C7	0.0430 (12)	0.0316 (9)	0.0404 (10)	−0.0034 (9)	0.0020 (9)	−0.0008 (8)
C8	0.0439 (12)	0.0344 (10)	0.0418 (10)	−0.0043 (9)	−0.0022 (10)	−0.0037 (8)

Geometric parameters (Å, º)

O1—C1	1.3913 (19)	C5—C6	1.387 (2)
O1—H1	0.90 (3)	C5—H5	0.9500
C1—C6	1.392 (2)	C6—C8	1.509 (3)
C1—C2	1.398 (2)	C7—H7A	0.9800
C2—C3	1.389 (2)	C7—H7B	0.9800
C2—C7	1.503 (3)	C7—H7C	0.9800
C3—C4	1.380 (3)	C8—H8A	0.9800
C3—H3	0.9500	C8—H8B	0.9800
C4—C5	1.385 (3)	C8—H8C	0.9800
C4—H4	0.9500		
C1—O1—H1	112.2 (15)	C5—C6—C1	118.05 (16)
O1—C1—C6	116.36 (15)	C5—C6—C8	121.06 (17)
O1—C1—C2	121.28 (16)	C1—C6—C8	120.88 (16)
C6—C1—C2	122.32 (16)	C2—C7—H7A	109.5
C3—C2—C1	117.38 (17)	C2—C7—H7B	109.5
C3—C2—C7	120.93 (17)	H7A—C7—H7B	109.5
C1—C2—C7	121.69 (16)	C2—C7—H7C	109.5
C4—C3—C2	121.58 (18)	H7A—C7—H7C	109.5
C4—C3—H3	119.2	H7B—C7—H7C	109.5
C2—C3—H3	119.2	C6—C8—H8A	109.5
C3—C4—C5	119.64 (18)	C6—C8—H8B	109.5
C3—C4—H4	120.2	H8A—C8—H8B	109.5
C5—C4—H4	120.2	C6—C8—H8C	109.5
C4—C5—C6	121.01 (19)	H8A—C8—H8C	109.5
C4—C5—H5	119.5	H8B—C8—H8C	109.5
C6—C5—H5	119.5		
O1—C1—C2—C3	−179.36 (17)	C3—C4—C5—C6	−0.7 (3)
C6—C1—C2—C3	−1.6 (2)	C4—C5—C6—C1	0.4 (3)
O1—C1—C2—C7	0.5 (3)	C4—C5—C6—C8	−179.23 (19)
C6—C1—C2—C7	178.23 (18)	O1—C1—C6—C5	178.60 (16)
C1—C2—C3—C4	1.4 (3)	C2—C1—C6—C5	0.8 (3)

C7—C2—C3—C4	−178.49 (18)	O1—C1—C6—C8	−1.8 (2)
C2—C3—C4—C5	−0.3 (3)	C2—C1—C6—C8	−179.61 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{i}	0.90 (3)	1.89 (3)	2.7470 (14)	158 (2)

Symmetry code: (i) *x*+1/2, −*y*+1/2, −*z*+2.