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4-(2-Phenylisopropyl)phenol

Abdelhak Ettahiri,[a]* Mostafa Abboudi,[a] Daphne Merle,[b] Monique Perrin[b] and Alain Thozet[b]

[a]Université Abdelmalek Essaadi, Faculté des Sciences Tetouan, Département Chimie, BP 2121 93000 Tetouan, Morocco, and [b]Centre de Diffractometrie, Université Claude Bernard Lyon 1, 43 boulevard du 11 Novembre 1918, 69622 Villeurbanne Cedex, France

Correspondence e-mail: ettahiri@fst.ac.ma

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.128
Data-to-parameter ratio = 19.4

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

The structure of 4-cumylphenol, $C_{15}H_{16}O$, exhibits chains of hydrogen-bonded molecules along the c axis.

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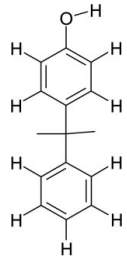
Comment

In the solid state, 4-cumylphenol, (I), crystallizes in space group $R\overline{3}$. The molecules are linked by hydrogen bonds, giving infinite chains along the c axis; van der Waals interactions between chains have distances of about 3.5 Å. *p*-Cumylphenol was used to synthesize calixarenes with four, six and eight arene units. These macrocycles trap solvent molecules (Gutsche, 1998; Perrin *et al.*, 2003). The conformation of the molecule shows that the two aromatic rings are nearly perpendicular [dihedral angle = 97.71 (5)°]. Atoms C14 and C15 lie 0.204 (3) and −1.588 (3) Å, respectively, from the plane of the phenol ring, and 0.708 (1) and −0.429 (1) Å from the plane of the cumyl ring. The C3—C4—C7—C8 torsion angle value is 47.71 (13)°. The unit cell contains 18 molecules, showing chains around the helicoidal 3_1 axes. One chain is formed with molecules linked by O—H···O hydrogen bonds as described in Table 1. This type of structure was reported for thymol (2-isopropyl-3-methylphenol; Thozet & Perrin, 1980), and the latter compound crystallized in the same space group. Interactions between chains are found both between phenol rings and between cumyl rings (values 3.51–3.59 Å).



(I)

Experimental

The title compound was obtained from a (Aldrich) and was dissolved in methanol. Slow evaporation gave single crystals of good quality for X-ray analysis.

Crystal data

$C_{15}H_{16}O$
M_r = 212.28
Rhombohedral, $R\overline{3}$
a = 30.989 (4) Å
c = 6.500 (1) Å
V = 5405.5 (13) Å^3
Z = 18
D_x = 1.174 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8097 reflections
θ = 1.0–27.9°
μ = 0.07 mm^{-1}
T = 150 (2) K
Prism, colorless
0.40 × 0.15 × 0.15 mm

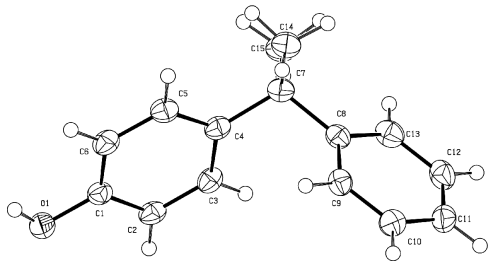


Figure 1
View of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Nonius KappaCCD diffractometer	$\theta_{max} = 27.9^\circ$
φ scans	$R_{int} = 0.075$
Absorption correction: none	$h = -40 \rightarrow 40$
15 965 measured reflections	$k = -40 \rightarrow 40$
2855 independent reflections	$l = -8 \rightarrow 8$
1948 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.049$	$+ 5.893P]$
$wR(F^2) = 0.129$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{max} = 0.004$
2855 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
147 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.83	1.88	2.710 (1)	173

Symmetry code: (i) $\frac{1}{3} - y, x - y - \frac{1}{3}, z - \frac{1}{3}$.

All H atoms were treated as riding on their parent atoms, with C—H distances of 0.94 (aromatic) and 0.97 Å (methyl), an O—H distance of 0.83 Å, and $U_{iso}(H) = 1.2U_{eq}(C_{aromatic})$ and $1.5U_{eq}(C_{methyl},O)$.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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