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trans-2-(2-Hydroxyphenyl)cyclohexanol

Kandasamy Chinnakali,[a] Thangavel Ravishankar,[b] Kamaraj Sriraghavan,[c] Ibrahim Abdul Razak,[d] Hoong-Kun Fun,[d]* Suchada Chantrapromma[d]† and Vayalakkavoor T. Ramakrishnan[c]

[a]Department of Physics, Anna University, Chennai 600025, India, [b]Department of Physics, Deen Dayal Engineering College, Kunnavalam 600210, Tamil Nadu, India, [c]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600025, India, and [d]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

† Permanent address: Department of Chemistry, Faculty of Science, Prince of Songkhla University, Hat-Yai, Songkhla 90112, Thailand.

Correspondence e-mail: hkfun@usm.my

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The crystal structure of the title compound, $C_{12}H_{16}O_2$, contains two crystallographically independent molecules in the asymmetric unit. The cyclohexane rings of these two molecules adopt chair conformations with the hydroxyl groups and benzene rings equatorially attached. The crystal structure is stabilized by O—H···O hydrogen bonds and weak C—H···π interactions involving the phenyl rings.

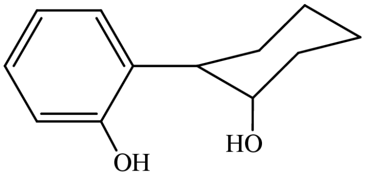
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.078
wR factor = 0.223
Data-to-parameter ratio = 13.6

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

Comment

Cyclohexanol and its derivatives have proven to be important tools in both biochemical and physiological studies of the cholimergin nerve terminal (Rogers *et al.*, 1989). Also, many of the cyclohexanol derivatives exhibit good receptor properties against the inhibitor of acetylcholine storage by nerve terminal synaptic vesicles (Marshall & Parsons, 1987). The crystal structure determination of the title compound, (I), one of the above derivatives, was performed in order to elucidate its molecular conformation.



(I)

The asymmetric unit of (I) contains two crystallographically independent molecules linked by an O1*B*—H1*C*···O2*A* hydrogen bond, with their centroid at (0.252, 0.250, 0.497). The corresponding bond lengths and angles of these two molecules agree with each other and show normal values. The cyclohexane ring in both molecules adopts the chair conformation and the hydroxyl and phenyl groups are equatorially attached. An O—H···O intramolecular hydrogen bond is observed in each of the two molecules in the asymmetric unit (Table 1). In the solid state, the two independent molecules are alternately linked by O—H···O hydrogen bonds to form an infinite one-dimensional chain along the *a* direction. The crystal structure is further stabilized by a number of weak C—H···π interactions involving the phenyl rings of molecule *A* (πP*A* = centroid of C1*A*–C6*A*) and molecule *B* (πP*B* = centroid of C1*B*–C6*B*).

Experimental

To a stirred suspension of magnesium turnings (0.75 g-atom) in dry THF (25 ml) under a nitrogen atmosphere was added dropwise a

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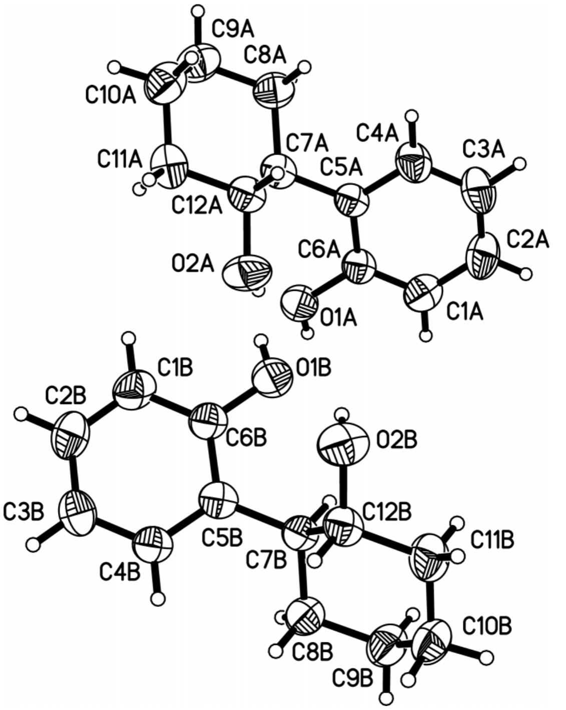

Figure 1
The structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

solution of 2-bromoanisole (3.8 ml, 0.03 *M*) in dry THF (15 ml). After the addition was complete, the solution was cooled to 263 K (using an ice–salt mixture), and cuprous iodide (0.29 g, 1.5 mmol) was added. The resulting mixture was then stirred for a further 15 min, after which time cyclohexane oxide (2 ml, 0.02 *M*) in dry THF (10 ml) was added dropwise. After completion of the reaction, it was quenched with a saturated solution of ammonium sulfate (50 ml). The reaction mixture was then extracted with ethyl acetate and the organic layer was washed with water, then dried over anhydrous $MgSO_4$. After removal of the solvent, the residue was chromatographed over silica gel to afford *trans*-2-(2-methoxyphenyl)cyclohexanol (4.1 g, 98%) as a viscous liquid in 98% yield. It was then further demethylated with chlorotrimethylsilane (2.17 g, 0.02 *M*) and sodium iodide (3 g, 0.02 *M*) using dry acetonitrile as solvent, affording the title compound as a crystalline solid (m.p. 367–369 K).

Crystal data

$C_{12}H_{16}O_2$
$M_r = 192.25$
Triclinic, $P\bar{1}$
$a = 9.0290$ (7) Å
$b = 10.0804$ (8) Å
$c = 12.1751$ (10) Å
$\alpha = 72.031$ (2)°
$\beta = 81.913$ (2)°
$\gamma = 89.545$ (2)°
$V = 1042.9$ (1) Å^3

$Z = 4$
$D_x = 1.224$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2614 reflections
$\theta = 1.8$–28.4°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Plate, colourless
0.48 × 0.40 × 0.14 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
5444 measured reflections
3503 independent reflections
1965 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.046$
$\theta_{\rm max} = 25.0°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = 0 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.078$
$wR(F^2) = 0.223$
$S = 0.96$
3503 reflections
257 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1210P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.29$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.32$ e Å^{-3}

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

*π*P*A* is the centroid of ring C1*A*–C6*A* and *π*P*B* is the centroid of ring C1*B*–C6*B*.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···O2*B*^{i}	0.82	1.87	2.655 (4)	159
O1*B*—H1*C*···O2*A*	0.82	1.86	2.661 (4)	167
O2*A*—H2*A*···O1*A*	0.82	2.01	2.803 (4)	163
O2*B*—H2*C*···O1*B*	0.82	2.11	2.817 (4)	144
C9*A*—H9*B*···*π*P*B*^{ii}	0.97	3.11	3.965 (5)	148
C9*B*—H9*D*···*π*P*A*^{iii}	0.97	3.06	3.924 (4)	149
C11*A*—H11*B*···*π*P*B*^{iv}	0.97	3.09	3.931 (4)	146
C11*B*—H11*C*···*π*P*A*^{v}	0.97	3.11	3.930 (4)	144

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

After checking their presence in the difference map, all the H atoms were placed in geometrically calculated positions and a riding model was used for their refinement. A rotating group refinement was used for the hydroxyl groups.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

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