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Crystal structure of (6-phenylcyclohex-3-enyl)methanol, $C_{13}H_{16}O$

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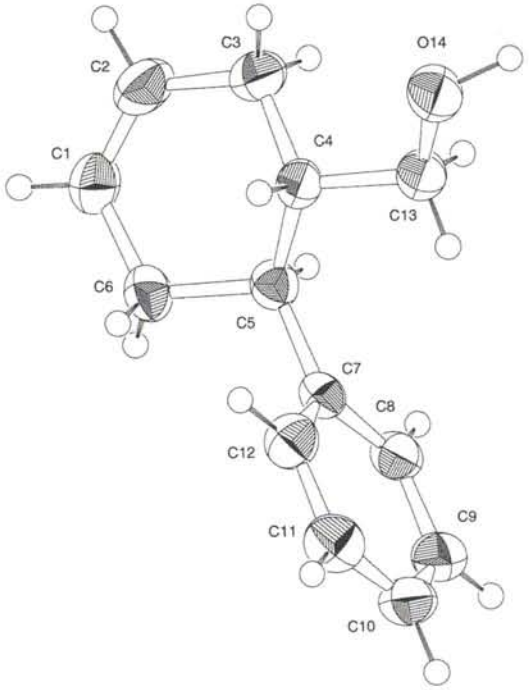

Abstract

$C_{13}H_{16}O$, monoclinic, *C*1*c*1 (No. 9), $a = 7.104(1)$ Å, $b = 28.784(1)$ Å, $c = 5.444(1)$ Å, $\beta = 106.21(1)°$, $V = 1069.0$ Å^3, $Z = 4$, $R(F) = 0.035$, $wR_{ref}(F^2) = 0.047$, $T = 298$ K.

Source of material

The title compound has been synthetized by reduction of 6-phenylcyclohex-3-ene carbaldehyde diluted in diethyl ether with $LiAlH_4$. After extraction, the crude compound was recrystallized in CH_2Cl_2.

Discussion

The compound adopts an half-chair conformation [1] for the cyclohexene ring with diequatorial substituants (C7C5C4C13 = 50.13(5)°). To minimize the steric interactions between the two substituants, the phenyl group P2(C7C8C9C10C11C12) make an angle of 86.73(4)° with the mean plane P1 of cyclohexene. There are strong intramolecular hydrogen bonds between *d*(O14—H4) = 2.490(3) Å, *d*(O14—H13A) = 1.965(3) Å and *d*(O14—H13B) = 1.980(3) Å.

In the packing, we observe a tetramer, stabilized by intermolecular hydrogen bonds *d*(O14—H14) = 1.9581(3) Å [symmetry code: $x, -y, z+1/2$] which is constituted by two dimers each ones stabilized by a stacking of the phenyl groups. The distance between the phenyl planes is (5.4444(3) Å) [symmetry code: x, y, z ; $x, -y, z+1/2$ and $x, y, z-1$; $x, -y, z-1/2$].

Table 1. Data collection and handling.

Crystal:	colourless prism, size 0.25 × 0.35 × 0.55 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	0.72 cm^{-1}
Diffractometer, scan mode:	Nonius Kappa CCD, φ
$2\theta_{max}$:	52.56°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1073, 1052
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\ \sigma(I_{obs})$, 1012
$N(param)_{refined}$:	125
Programs:	SIR92 [2], MAXUS [3], ORTEPII [5],

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{iso}
H(5)	4*a*	1.2325	0.1365	0.7854	0.05
H(4)	4*a*	1.0369	0.0693	0.9895	0.05
H(8)	4*a*	1.0523	0.1950	0.5325	0.05
H(13A)	4*a*	0.8608	0.0850	0.5616	0.05
H(13B)	4*a*	1.0452	0.0685	0.4807	0.05
H(6A)	4*a*	1.1752	0.1400	1.2712	0.05
H(6B)	4*a*	1.3169	0.1719	1.1730	0.05
H(3A)	4*a*	1.3493	0.0540	0.7852	0.05
H(3B)	4*a*	1.2668	0.0186	0.9478	0.05
H(9)	4*a*	0.7802	0.2440	0.4053	0.05
H(12)	4*a*	0.8309	0.1367	1.0644	0.05
H(11)	4*a*	0.5562	0.1863	0.9404	0.05
H(10)	4*a*	0.5312	0.2401	0.6114	0.05
H(2)	4*a*	1.5521	0.0477	1.2398	0.05
H(1)	4*a*	1.5254	0.1173	1.4248	0.05
H(14)	4*a*	0.8810	0.0031	0.4406	0.05

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(14)	4*a*	0.91000(9)	0.01794(1)	0.611000(9)	0.0747(3)	0.0343(2)	0.0504(2)	–0.0059(2)	0.0026(2)	–0.0037(2)
C(7)	4*a*	0.96895(9)	0.16122(2)	0.8104(1)	0.0380(3)	0.0314(2)	0.0348(3)	–0.0009(2)	0.0083(2)	–0.0057(2)
C(5)	4*a*	1.14851(9)	0.13038(2)	0.8926(1)	0.0398(3)	0.0361(3)	0.0347(3)	–0.0012(2)	0.0110(2)	0.0000(2)
C(4)	4*a*	1.1048(1)	0.07803(2)	0.8668(1)	0.0440(3)	0.0349(3)	0.0341(3)	0.0007(2)	0.0040(2)	0.0007(2)
C(8)	4*a*	0.9493(1)	0.19353(2)	0.6150(1)	0.0522(3)	0.0351(2)	0.0404(3)	0.0023(2)	0.0187(2)	–0.0005(2)
C(13)	4*a*	0.9732(1)	0.06490(2)	0.6048(1)	0.0602(4)	0.0324(2)	0.0412(3)	0.0005(2)	0.0009(3)	–0.0017(2)
C(6)	4*a*	1.2657(1)	0.14097(2)	1.1693(1)	0.0441(3)	0.0444(3)	0.0392(3)	–0.0056(2)	0.0062(2)	–0.0072(2)
C(3)	4*a*	1.2962(1)	0.05070(2)	0.9283(1)	0.0534(3)	0.0402(3)	0.0535(3)	0.0073(3)	0.0046(3)	0.0017(3)
C(9)	4*a*	0.7881(1)	0.22218(2)	0.5413(1)	0.0638(4)	0.0374(3)	0.0451(3)	0.0082(3)	0.0156(3)	0.0020(2)
C(12)	4*a*	0.8192(1)	0.15898(2)	0.9296(1)	0.0473(3)	0.0442(3)	0.0430(3)	–0.0014(2)	0.0150(3)	0.0046(2)
C(11)	4*a*	0.6579(1)	0.18819(2)	0.8560(2)	0.0390(3)	0.0570(3)	0.0584(4)	–0.0007(3)	0.0192(3)	–0.0040(3)
C(10)	4*a*	0.6425(1)	0.2198(2)	0.6613(1)	0.0469(3)	0.0424(3)	0.0564(3)	0.0099(3)	0.0084(3)	–0.0031(3)
C(2)	4*a*	1.4430(1)	0.06762(2)	1.1634(2)	0.0447(3)	0.0566(3)	0.0648(4)	0.0107(3)	–0.0035(3)	0.0037(3)
C(1)	4*a*	1.4284(1)	0.10771(2)	1.2722(1)	0.0477(4)	0.0582(4)	0.0487(3)	0.0002(3)	–0.0061(3)	–0.0058(3)

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