Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(Cyclohexyliminomethyl)phenol

Wu Li, Tao Zeng* and Yang Li

School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China

Correspondence e-mail: zengtaotj@126.com

Received 21 June 2006
Accepted 14 July 2006

The title compound, $C_{13}H_{17}NO$, was prepared by reductive amination from 4-hydroxybenzaldehyde and cyclohexanamine. The crystal packing is stabilized by O—H···N hydrogen bonds.

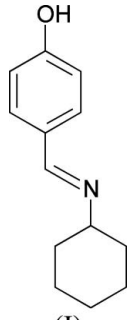
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.116
Data-to-parameter ratio = 14.7

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

Comment

Schiff base derivatives are widely synthesized *via* reductive amination reactions. Recently we have reported the synthesis and crystal structure of a new Schiff base compound with a hindered phenol group (Yan *et al.*, 2006). As part of our ongoing research in this field, the title compound, (I), has been prepared by reductive amination from 4-hydroxybenzaldehyde and cyclohexanamine, and its crystal structure is reported here.



(I)

In (I), bond lengths and angles are as expected for a molecule of this kind (Allen *et al.*, 1987). The cyclohexyl ring adopts a chair conformation with puckering parameters Q = 0.554 (2) Å, φ_2 = −85.4 (8)° and θ_2 = 178.6 (2)° (Cremer & Pople, 1975).

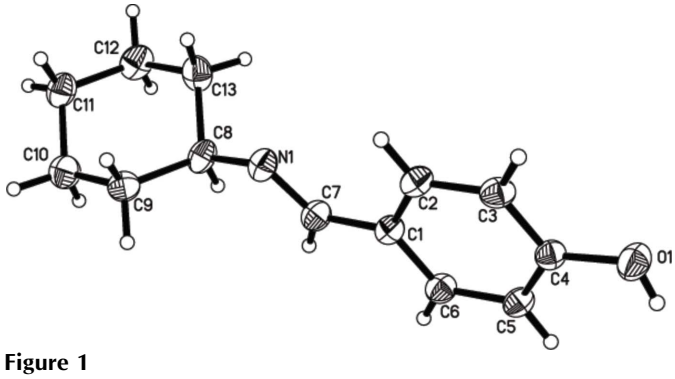


Figure 1
A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

© 2006 International Union of Crystallography
All rights reserved

The crystal structure is stabilized by intermolecular O—H···N hydrogen bonds (Table 1).

Experimental

A mixture of 4-hydroxybenzaldehyde (6.1 g, 0.05 mol) and cyclohexanamine (4.95 g, 0.05 mol) in toluene (100 ml) was heated at 383 K and refluxed for 4 h. The solvent was then evaporated under reduced pressure to afford the title compound in 98% yield (9.96 g). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane/ethanol solution (6:1 *v*/*v*; m.p. 446–448 K).

Crystal data

$C_{13}H_{17}NO$
$M_r = 203.28$
Monoclinic, $P2_1/n$
$a = 5.6582\ (16)$ Å
$b = 17.453\ (5)$ Å
$c = 11.833\ (3)$ Å
$\beta = 97.102\ (5)^\circ$
$V = 1159.5\ (6)$ Å^3
$Z = 4$
$D_x = 1.164$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 294\ (2)$ K
Block, colourless
0.26 × 0.24 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.981$, $T_{max} = 0.984$
5807 measured reflections
2043 independent reflections
1346 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.116$
$S = 1.04$
2043 reflections
139 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.1411P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.13$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.94 (2)	1.83 (2)	2.755 (2)	168 (2)

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

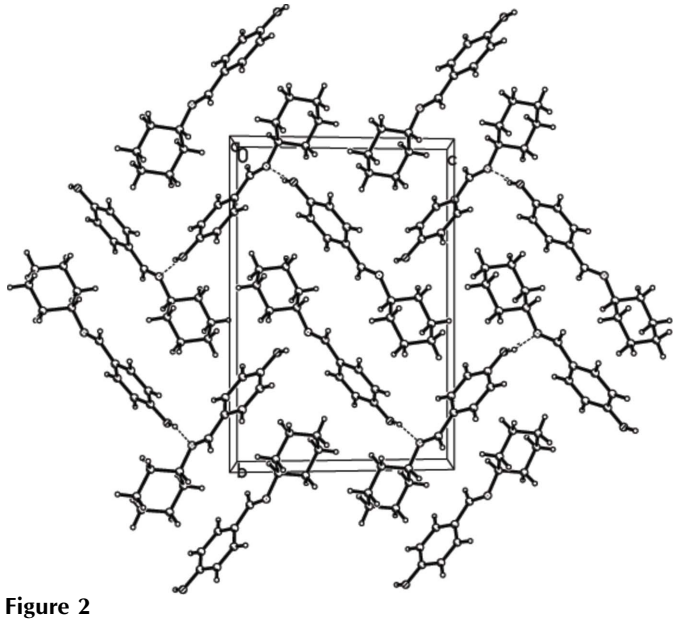


Figure 2
Packing diagram of (I) viewed along the *a* axis, showing the intermolecular O—H···N hydrogen interactions (dashed lines).

The H atom of the hydroxy group was located in a difference Fourier map and refined with the O—H distance restrained to 0.82Å. All other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.98 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yan, X.-L., Chen, L.-G. & Zeng, T. (2006). *Acta Cryst.* E**62**, o1455–o1456.