Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(2-Chlorophenyl)cyclohexanecarbonitrile

Andreas Lemmerer* and Joseph P. Michael

Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, PO Wits 2050, South Africa

Correspondence e-mail: anderl@chem.wits.ac.za

Received 20 December 2006
Accepted 18 January 2007

In the title compound, $C_{13}H_{14}ClN$, the cyclohexane ring adopts a chair conformation with an axial nitrile substituent. Intermolecular Ar—H···N bridges stabilize the crystal packing.

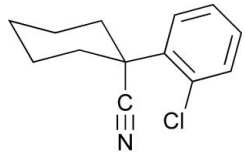
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.098
Data-to-parameter ratio = 20.3

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

Comment

The title compound, (I), was prepared as part of a model study to identify suitable precursors for the construction of oxindoles bearing spirocyclic rings at C3 (Fleming *et al.*, 1982, 1986). These spiro-oxindoles in turn served as models in the development of a methodology aimed at the total synthesis of the complex spiro-oxindole alkaloid gelsemine (Clarke *et al.*, 1988).



(I)

The molecular structure of (I) shows that the cyclohexane ring is in the expected chair conformation, with the nitrile group adopting an axial orientation (Fig. 1). The crystal structure of (I) is built-up by weak intermolecular Ar—H···N hydrogen bonds (Table 1) that link the molecules into chains with a $C(7)$ motif (Etter *et al.*, 1990; Bernstein *et al.*, 1995) running parallel to the [010] direction (Fig. 2).

Experimental

The title compound was prepared as described previously by alkylation of (2-chlorophenyl)acetonitrile with 1,5-dibromopentane in

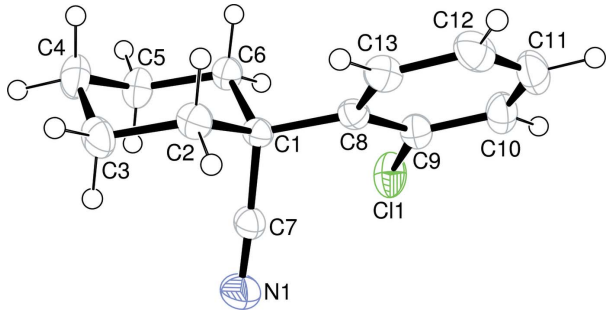


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

dimethyl sulfoxide in the presence of potassium hydroxide (Fleming *et al.*, 1986). Crystals suitable for X-ray crystallography were obtained as colourless plates by recrystallization from a mixture of chloroform and hexane (1:1).

Crystal data

$C_{13}H_{14}ClN$
$M_r = 219.7$
Monoclinic, $P2_1/c$
$a = 7.7680\ (5)$ Å
$b = 11.9121\ (9)$ Å
$c = 12.9065\ (8)$ Å
$\beta = 107.129\ (4)^\circ$
$V = 1141.31\ (13)$ Å^3
$Z = 4$
$D_x = 1.279$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.3$ mm^{-1}
$T = 173\ (2)$ K
Plate, colourless
0.50 × 0.50 × 0.08 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
ω scans
Absorption correction: Gaussian (*SAINT-Plus*; Bruker, 1999)
$T_{min} = 0.864$, $T_{max} = 0.976$
9233 measured reflections
2762 independent reflections
2247 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 28.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.098$
$S = 1.05$
2762 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.1882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···N1^{i}	0.95	2.61	3.4003 (19)	141

Symmetry code: (i) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were positioned geometrically and allowed to ride on their respective parent atoms, with C—H = 0.95 (aromatic CH) or 0.99 Å (methylene CH_2), and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART-NT* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2003).

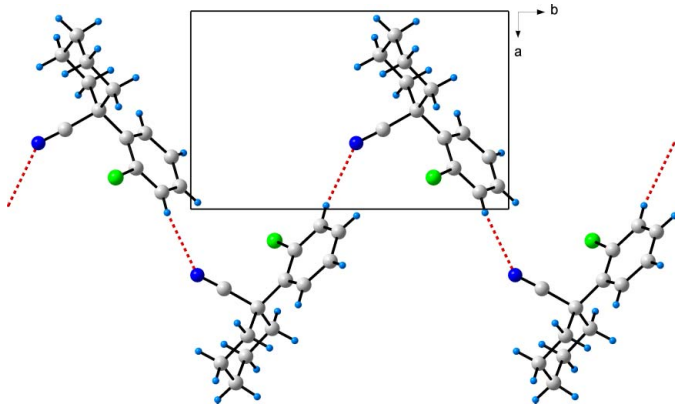


Figure 2
Packing diagram of (I), viewed along the *c* axis. Intermolecular Ar—H···N hydrogen bridges are shown as dotted red lines.

This work was supported by grants from the National Research Foundation, Pretoria (NRF, GUN 2053652 and GUN 2069064) and the University of the Witwatersrand.

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Brandenburg, K. (1999). *DIAMOND*. Version 2.1e. Crystal Impact GbR, Bonn, Germany.
Bruker (1998). *SMART-NT*. Version 5.050. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT-Plus*. Version 6.02, including *XPREP*. Bruker AXS Inc., Madison, Wisconsin, USA.
Clarke, C., Fleming, I., Fortunak, J. M. D., Gallagher, P. T., Honan, M. C., Mann, A., Nübling, C. O., Raithby, P. R. & Wolff, J. J. (1988). *Tetrahedron*, **44**, 3931–3944.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Fleming, I., Loreto, M. A., Michael, J. P. & Wallace, I. H. M. (1982). *Tetrahedron Lett.* **23**, 2053–2056.
Fleming, I., Loreto, M. A., Wallace, I. H. M. & Michael, J. P. (1986). *J. Chem. Soc. Perkin Trans. 1*, pp. 349–359.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.