Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(2-Bromophenyl)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

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.072
Data-to-parameter ratio = 20.7

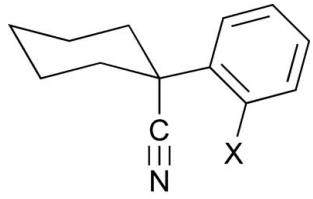
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 January 2007
Accepted 18 January 2007

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

Comment

The title compound, (I), was prepared together with its chloro and fluoro analogues as starting materials for the synthesis of spiro[cyclohexane-1,3′-indol]-2′(1′*H*)-one, a model for several spirocyclic oxindole alkaloids (Fleming *et al.*, 1982, 1986). The crystal structure of the chloro analogue, (II), is reported in the preceding article (Lemmerer & Michael, 2007).



(I) X = Br
(II) X = Cl

The molecular structure of (I) is isomorphous to (II) and shows that the cyclohexane ring is in the same 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 (Fig. 2 and Table 1) that link the molecules into chains, with the graph-set notation $C(7)$ (Etter *et al.*, 1990; Bernstein *et al.*, 1995). The donor–acceptor separations are 2.62 and 2.61 Å, respectively, for (I) and (II).

Experimental

Compound (I) was prepared by alkylating (2-bromophenyl)acetonitrile with 1,5-dibromopentane in dimethyl sulfoxide at room temperature in the presence of potassium hydroxide, as described previously (Fleming *et al.*, 1986). Recrystallization from a mixture of chloroform and hexane (approximately 1:1) afforded crystals suitable for X-ray crystallography as colourless plates.

Crystal data

$C_{13}H_{14}BrN$
M_r = 264.16
Monoclinic, $P2_1/c$
a = 7.8650 (9) Å
b = 11.7892 (14) Å
c = 13.1101 (13) Å
β = 106.531 (5)°
V = 1165.3 (2) Å^3
Z = 4
D_x = 1.506 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 3.49 mm^{-1}
T = 173 (2) K
Plate, colourless
0.6 × 0.3 × 0.1 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
ω scans
Absorption correction: Gaussian (*SAINT-Plus*; Bruker, 1999)
T_{min} = 0.243, T_{max} = 0.715
7389 measured reflections
2821 independent reflections
2220 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 28.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.072
S = 0.98
2821 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0406P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 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	2.62	3.449 (3)	146

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).

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.

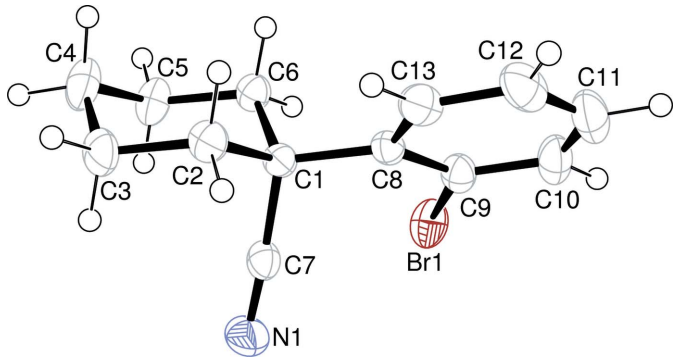


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

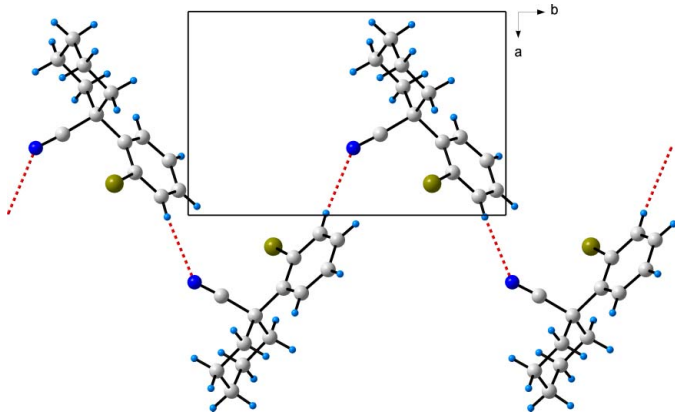


Figure 2
Packing diagram of (I), viewed along the *c* axis. Intermolecular Ar—H···N hydrogen bridges are shown as dotted red lines.

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.
Lemmerer, A. & Michael, J. P. (2007). *Acta Cryst.* E**63**, o916–o917.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.