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2,6-Dibromo-4-chlorobenzonitrile

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.057
Data-to-parameter ratio = 15.9

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

2,6-Dibromo-4-chlorobenzonitrile, $C_7H_2Br_2ClN$, forms layers in the crystal structure, with Br···N contacts of 3.049 (2) Å the strongest intermolecular interactions. The crystal structure is isomorphous with 2,4,6-tribromobenzonitrile.

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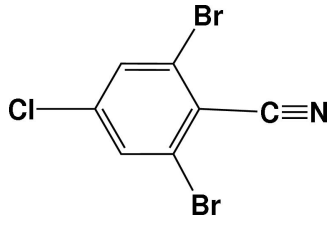
Comment

Previously, the structure of 2,6-dibromo-4-chlorobenzonitrile (Britton *et al.*, 2002) was found to be isomorphous with 2,4,6-tribromobenzonitrile (Carter & Britton, 1972), based on the similarities between the cell dimensions. The structure has been determined in full to obtain a precise measurement of the short Br···N distance that was expected in the structure.



(I)

Fig. 1 shows the labeling and the anisotropic displacement ellipsoids. The bond lengths and angles are normal.

Fig. 2 shows the packing. The molecules form layers that are virtually identical with those in the tribromo analog. The Br···N contacts are 3.049 (2) Å, with C—Br···N = 166.0 (2)° and Br···N—C = 133.2 (3)°. This is consistent with other structures in which Br acts as a Lewis acid and N acts as a bifurcated Lewis base. There are also H···Cl contacts, with H···Cl = 3.08 (3) Å, C—H···Cl = 16 (2)° and H···Cl—C = 100 (2)°; the angles are consistent with a C—H···Cl hydrogen

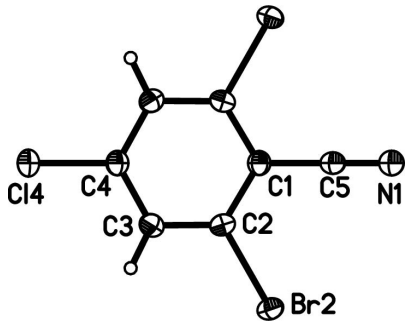


Figure 1
View of the title compound, with displacement ellipsoids shown at the 50% probability level. Unlabeled atoms are related to labeled atoms by $(x, \frac{1}{2}-y, z)$.

bond although the distance is slightly larger than the usual van der Waals distance for H···Cl (Bondi, 1964).

The layers are parallel to (20$\bar{1}$) with the molecules tilted by 1.4 (1)° out of the layer. Adjacent layers are 3.318 (1) Å apart.

Experimental

The compound was prepared from the corresponding aniline *via* the Sandmeyer reaction. [For details of the preparation of the tribromo isomorph, see Carter & Britton (1972).]

Crystal data

$C_7H_2Br_2ClN$	D_x = 2.346 Mg m^{-3}
M_r = 295.37	Mo $K\alpha$ radiation
Monoclinic, $P2_1/m$	Cell parameters from 2165 reflections
a = 8.666 (2) Å	θ = 2.4–27.4°
b = 10.125 (3) Å	μ = 9.94 mm^{-1}
c = 4.7776 (12) Å	T = 173 (2) K
β = 93.98 (1)°	Needle, colorless
V = 418.19 (19) Å^3	0.45 × 0.15 × 0.10 mm
Z = 2	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	1001 independent reflections
	930 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.024
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)	θ_{max} = 27.5°
	$h = -11 \rightarrow 5$
	$k = -13 \rightarrow 13$
T_{min} = 0.19, T_{max} = 0.37	$l = -6 \rightarrow 6$
2839 measured reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.25P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.022	
$wR(F^2)$ = 0.057	
S = 1.09	$(\Delta/\sigma)_{max}$ = 0.002
1001 reflections	$\Delta\rho_{max}$ = 0.43 e Å^{-3}
63 parameters	$\Delta\rho_{min}$ = −0.39 e Å^{-3}
All H-atom parameters refined	Extinction correction: *SHELXTL*
	Extinction coefficient: 0.047 (3)

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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*.

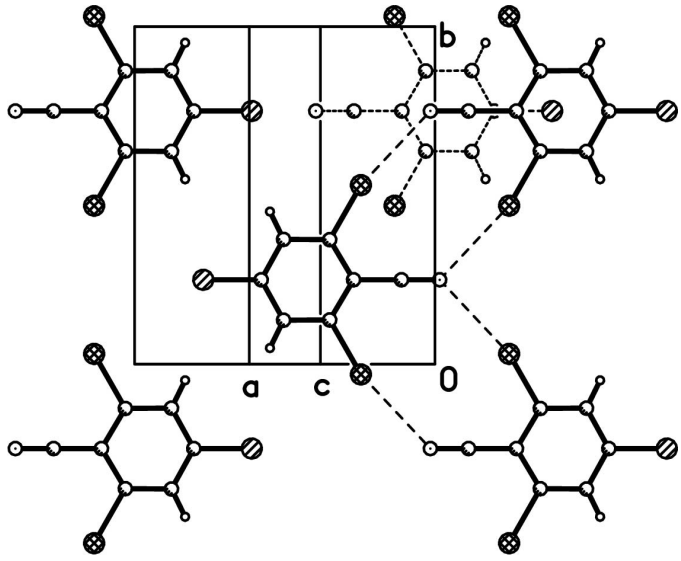


Figure 2
The packing in 2,6-dibromo-4-chlorobenzonitrile, viewed normal to (20$\bar{1}$). The molecules in one layer are shown with heavy bonds and the Br···N contacts are shown with dashed lines. One molecule in an adjacent layer is shown with dashed bonds.

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References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.
Britton, D., Noland, W. E. & Henke, T. A. (2002). *Acta Cryst.* E**58**, o185–o187.
Bruker (2002). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Carter, V. B. & Britton, D. (1972). *Acta Cryst.* B**28**, 945–950.
Sheldrick. G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.