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2-Chlorobiphenyl-4′-carbonitrile

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Abstract. $C_{13}H_8ClN$, $M_r = 213{\cdot}7$, monoclinic, $P2_1/c$, $a = 6{\cdot}78$ (4), $b = 23{\cdot}51$ (5), $c = 7{\cdot}25$ (2) Å, $\beta = 115{\cdot}3$ (2)°, $V = 1045$ Å^3, $Z = 4$, $D_m = 1{\cdot}32$, $D_x = 1{\cdot}36$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 2{\cdot}8$ mm^{-1}, $F(000) = 440$, $T = 293$ K, $R = 0{\cdot}046$ for 843 observed densitometer-measured equi-inclination Weissenberg data. The average C–C bond in the phenyl rings is 1·374 Å. The molecule is non-planar; the angle between the phenyl rings is 52·1 (1)°; the C–Cl bond is 1·731 (5) Å; the C–C ≡ N bonds are 1·421 (8) and 1·133 (7) Å, the C–C bond making an angle of 1·94 (6)° with the phenyl plane.

Introduction. The structure determination of the title compound forms part of an investigation into liquid-crystal compounds and their chemical precursors.

Experimental. D_m measured by flotation in aqueous cadmium *n*-dodecatungstoborate. Pale-yellow opaque crystals used in data collection about **c** and **a** had dimensions of 0·09 × 0·07 × 0·27 and 0·16 × 0·08 × 0·14 mm, respectively. 2574 reflections measured by the SERC Microdensitometer Service, Daresbury Laboratory, from multiple-film photographs using Cu $K\alpha$ radiation, 1989 unique, $-8 \le h \le 7$; $0 \le k \le 28$; $0 \le l \le 7$; 843 unique observed reflections; $R_{int} = 0{\cdot}05$. Structure solved by Patterson synthesis and refined (on F) by full-matrix least squares with anisotropic thermal parameters for the non-H atoms, H-atom positions, initially obtained from a difference synthesis and placed at geometrically reasonable positions, refined with constrained C–H bond distances and isotropic thermal parameters, final $R = 0{\cdot}046$, $w = 1/[\sigma^2(F) + 0{\cdot}005\,F^2]$,

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$wR = 0.070$. $(\Delta/\sigma)_{max}$ in final refinement cycle 0·02 for positional and 0·06 for thermal parameters. Max. and min. heights in final $\Delta\rho$ map +0·2 and −0·3 e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Computer programs used: *SHELX*76 (Sheldrick, 1976) and locally written programs supplied by HHS and Drs C. Morgan and M. J. Mottram.

Discussion. Table 1* gives atomic parameters and Table 2 bond lengths. The atomic numbering is shown in Fig. 1. The phenyl rings are planar to within +0·011 Å, with an average C—C bond of 1·376 Å. Cl—C(2) [1·731 (5) Å] is slightly longer than the 1·723 (10) Å found in 3-chlorobiphenyl-4-carbonitrile (Sutherland & Rawas, 1984), and shorter than the 1·745 (6) Å in 4-acetyl-3′-chlorobiphenyl (Sutherland, Rawas & Mottram, 1985). The Cl atom is displaced by 0·059 (3) Å from the phenyl ring, C(7) is displaced by 0·061 (5), C(13) by 0·048 (6) and N by 0·105 (6) Å with the C(13)—C(10) bond being inclined at 1·94 (6)° to the phenyl ring. The bond lengths of 1·421 (8) and 1·133 (7) Å for C(10)—C(13) and C(13)—N respectively are in agreement with the values of 1·438 (14) and 1·140 (16) Å for the corresponding bonds in 3-chlorobiphenyl-4-carbonitrile. The angles C(9)—C(10)—C(11), C(9)—C(10)—C(13), C(11)—C(10)—C(13) and C(10)—C(13)—N, of 120·6 (5), 120·4 (5), 119·0 (5) and 178·6 (6)°, compare with the corresponding angles of 118·5 (9), 120·5 (9), 121·0 (10) and 178·9 (13)° in 3-chlorobiphenyl-4-carbonitrile.

The angle between the phenyl rings about the central C—C bond, φ_1, of 52·1 (1)° is slightly larger than the 49·2 (10)° in 4-acetyl-2′-chlorobiphenyl (Sutherland & Hoy, 1968); the axis of the molecule defined by C(1), C(4), C(7), C(10) deviates from collinearity. Not only is there rotation φ_1 about the C(1)—C(7) bond but also $\varphi_2 = 2.4$ (7)° for the rotation of the ring C(1)—C(6) about an axis in its plane through C(1) perpendicular to C(1)—C(7), and $\varphi_3 = 1.1$ (6)°, the corresponding angle of rotation for ring C(7)—C(12).

There are six intermolecular contacts less than 3·7 Å excluding hydrogen atoms, of which the shortest are 3·520 (6) Å from C(8) to N at x, y, $z-1$ and 3·558 (5) Å between C(4) and Cl at $x-1$, $1.5-y$, $z-0.5$.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, bond angles, mean-plane calculations and intermolecular contact distances have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43839 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional coordinates* (×10^4) *and equivalent isotropic thermal parameters* (Å^2 ×10^4) *with e.s.d.'s in parentheses*

$U_{eq} = (U_{11}U_{22}U_{33})^{1/3}$.

	x	y	z	U_{eq}
Cl	7604 (2)	8067 (1)	2656 (2)	712 (7)
C(1)	3670 (7)	8550 (2)	1713 (7)	430 (25)
C(2)	4861 (8)	8179 (2)	1130 (8)	490 (27)
C(3)	3961 (10)	7866 (2)	−613 (9)	619 (37)
C(4)	1782 (10)	7919 (2)	−1849 (9)	608 (40)
C(5)	534 (10)	8284 (2)	−1345 (9)	592 (32)
C(6)	1458 (8)	8595 (2)	428 (8)	522 (28)
C(7)	4570 (7)	8874 (2)	3631 (7)	427 (26)
C(8)	6395 (8)	9210 (2)	4176 (7)	484 (28)
C(9)	7221 (8)	9499 (2)	5981 (8)	505 (28)
C(10)	6218 (8)	9456 (2)	7281 (8)	467 (29)
C(11)	4368 (9)	9135 (2)	6756 (9)	586 (32)
C(12)	3558 (9)	8841 (2)	4942 (8)	538 (31)
C(13)	7095 (9)	9743 (2)	9188 (9)	545 (30)
N	7820 (8)	9963 (2)	10726 (9)	717 (30)

Table 2. *Bond lengths* (Å) *with e.s.d.'s in parentheses*

Cl—C(2)	1·731 (5)	C(7)—C(8)	1·377 (6)
C(1)—C(2)	1·373 (7)	C(8)—C(9)	1·364 (7)
C(2)—C(3)	1·361 (8)	C(9)—C(10)	1·381 (8)
C(3)—C(4)	1·368 (8)	C(10)—C(11)	1·372 (7)
C(4)—C(5)	1·360 (8)	C(11)—C(12)	1·374 (7)
C(5)—C(6)	1·376 (8)	C(7)—C(12)	1·391 (7)
C(1)—C(6)	1·391 (6)	C(10)—C(13)	1·421 (8)
C(1)—C(7)	1·469 (6)	C(13)—N	1·133 (7)

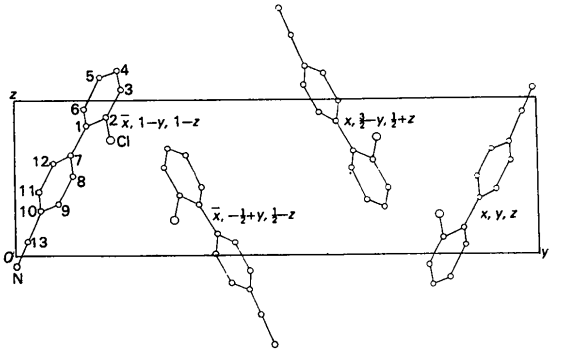

Fig. 1. The arrangement of molecules in the unit cell viewed along **a**.

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