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N-(3,4-Dichlorophenyl)benzamide

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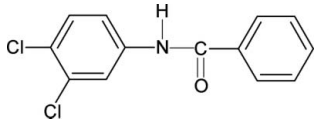
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.093; data-to-parameter ratio = 15.0.

The conformation of the N—H bond in the structure of the title compound, $C_{13}H_9Cl_2NO$, is *anti* to the *meta*-chloro substituent in the dichlorophenyl ring, similar to that observed with respect to the *meta*-chloro substituent in *N*-(3,4-dichlorophenyl)acetamide and *ortho*-chloro substituent in *N*-(2-chlorophenyl)benzamide, but in contrast to the *syn* conformation observed with respect to both the *ortho*-chloro and *meta*-chloro substituents in *N*-(2,3-dichlorophenyl)-benzamide. The bond parameters are similar to those in 2-chloro-*N*-phenylbenzamide, *N*-(2-chlorophenyl)benzamide and *N*-(2,3-dichlorophenyl)benzamide. The molecules are packed into chains in the direction of the *b* axis through N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2003); Gowda, Kozisek *et al.* (2007); Gowda, Sowmya, Kožíšek *et al.* (2007); Gowda, Sowmya, Tokarcik *et al.* (2007); Jones *et al.* (1990); Clark & Reid (1995).



Experimental

Crystal data

$C_{13}H_9Cl_2NO$
M_r = 266.11
Monoclinic, $P2_1/c$
a = 11.2828 (2) Å
b = 5.1400 (1) Å
c = 20.9368 (5) Å
β = 103.657 (2)°
V = 1179.87 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 295 (2) K
0.32 × 0.09 × 0.05 mm

Data collection

Oxford Diffraction Xcalibur System diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.811, T_{max} = 0.963
18488 measured reflections
2316 independent reflections
1788 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.093
S = 1.07
2316 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.16	2.9568 (19)	153

Symmetry code: (i) $x, y-1, z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2417).

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supplementary materials

Acta Cryst. (2007). E**63**, o3365 [**doi:10.1107/S1600536807031571**]

N-(3,4-Dichlorophenyl)benzamide

B. T. Gowda, B. P. Sowmya, M. Tokarcík, J. Kozísek and H. Fuess

Comment

In the present work, the structure of *N*-(3,4-dichlorophenyl)-benzamide has been determined to explore the substituent effects on the structures of N-aromatic amides (Gowda *et al.*, 2003; Gowda, Kozisek *et al.*, 2007; Gowda, Sowmya, Kožíšek *et al.* 2007; Gowda, Sowmya, Tokarcik *et al.*, 2007). The conformation of the N—H bond (Fig. 1) is anti to the *meta*-chloro substituent in the aniline phenyl ring, similar to that observed with respect to the *meta* chloro substituent in *N*-(3,4-dichlorophenyl)-acetamide (Jones *et al.*, 1990) and *ortho* chloro substituent in *N*-(2-chlorophenyl)-benzamide (Gowda, Sowmya, Kožíšek *et al.* 2007), but in contrast to the *syn* conformation observed with respect to both the *ortho*-chloro and *meta*-chloro substituents in *N*-(2,3-dichlorophenyl)-benzamide (Gowda, Sowmya, Tokarcik *et al.*, 2007). The bond parameters are similar to those in *N*-(phenyl)-2-chlorobenzamide (Gowda *et al.*, 2003), *N*-(2-chlorophenyl)-benzamide (Gowda, Sowmya, Kožíšek *et al.* 2007) and *N*-(2,3-dichlorophenyl)-benzamide (Gowda, Sowmya, Tokarcik *et al.*, 2007). Hydrogen bond link the molecules to chains running along the *b* axis (Fig.2).

Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra. Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

Refinement

H atoms were seen in difference map and refined using a riding model with C–H distances 0.93Å for the ring hydrogen atoms, 0.86Å for the H(N) atom, and with U_{iso}(H) = 1.2 U_{eq}(C) for all H atoms.

Figures

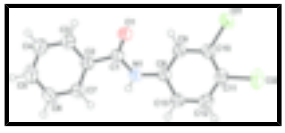

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

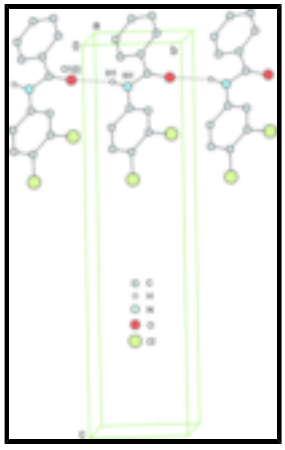

Fig. 2. Part of crystal structure of the title; hydrogen bonds shown as dashes lines. H atoms not involved in hydrogen bonding have been omitted. Symmetry code (i): $x, y-1, z$.

N-(3,4-Dichlorophenyl)benzamide

Crystal data

$C_{13}H_9Cl_2NO$	F_{000} = 544
M_r = 266.11	D_x = 1.498 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7847 reflections
a = 11.2828 (2) Å	θ = 3.6–29.5º
b = 5.1400 (1) Å	μ = 0.53 mm^{-1}
c = 20.9368 (5) Å	T = 295 (2) K
β = 103.657 (2)º	Prism, colorless
V = 1179.87 (4) Å^3	0.32 × 0.09 × 0.05 mm
Z = 4	

Data collection

Oxford Diffraction Xcalibur System diffractometer	1788 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 295(2) K	θ_{max} = 26.0º
ω scans with κ offsets	θ_{min} = 4.1º
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2006)	h = −13→13
T_{min} = 0.811, T_{max} = 0.963	k = −5→6
18488 measured reflections	l = −25→25
2316 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.033	H-atom parameters constrained

$wR(F^2) = 0.093$	$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.3587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
2316 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.06707 (16)	0.6618 (3)	0.07436 (9)	0.0408 (4)
C2	−0.17812 (16)	0.6102 (3)	0.02116 (9)	0.0403 (4)
C3	−0.20601 (19)	0.7783 (4)	−0.03154 (10)	0.0517 (5)
H3	−0.1533	0.9145	−0.0345	0.062*
C4	−0.3116 (2)	0.7460 (5)	−0.07990 (11)	0.0657 (6)
H4	−0.3293	0.8602	−0.1153	0.079*
C5	−0.3899 (2)	0.5489 (5)	−0.07623 (11)	0.0650 (6)
H5	−0.4607	0.5277	−0.1092	0.078*
C6	−0.3641 (2)	0.3810 (4)	−0.02368 (12)	0.0662 (6)
H6	−0.4181	0.2474	−0.0208	0.079*
C7	−0.25851 (19)	0.4096 (4)	0.02470 (11)	0.0557 (5)
H7	−0.2411	0.2941	0.0599	0.067*
C8	0.07957 (16)	0.4545 (3)	0.16650 (9)	0.0400 (4)
C9	0.17486 (16)	0.6320 (3)	0.17660 (9)	0.0437 (4)
H9	0.1784	0.7555	0.1446	0.052*
C10	0.26459 (16)	0.6244 (3)	0.23455 (9)	0.0446 (4)
C11	0.25928 (17)	0.4446 (4)	0.28304 (9)	0.0452 (4)
C12	0.16527 (18)	0.2642 (4)	0.27169 (10)	0.0498 (5)
H12	0.1622	0.1393	0.3034	0.06*
C13	0.07682 (17)	0.2684 (4)	0.21419 (9)	0.0455 (4)
H13	0.0145	0.1457	0.2071	0.055*
N1	−0.01460 (13)	0.4513 (3)	0.10875 (7)	0.0438 (4)
H1	−0.0414	0.3012	0.0939	0.053*
O1	−0.02755 (13)	0.8827 (2)	0.08692 (7)	0.0553 (4)
Cl1	0.38564 (5)	0.83887 (10)	0.24432 (3)	0.06298 (19)

Cl2	0.36741 (5)	0.43840 (12)	0.35648 (3)	0.0683 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0444 (10)	0.0324 (9)	0.0443 (10)	−0.0021 (8)	0.0079 (8)	−0.0013 (7)
C2	0.0415 (10)	0.0337 (9)	0.0444 (10)	0.0007 (7)	0.0077 (8)	−0.0044 (7)
C3	0.0554 (12)	0.0465 (11)	0.0502 (11)	−0.0031 (9)	0.0065 (9)	0.0026 (9)
C4	0.0719 (15)	0.0642 (14)	0.0517 (12)	0.0027 (12)	−0.0041 (11)	0.0066 (11)
C5	0.0529 (13)	0.0624 (14)	0.0672 (14)	0.0036 (11)	−0.0109 (10)	−0.0110 (11)
C6	0.0482 (12)	0.0563 (13)	0.0852 (16)	−0.0118 (10)	−0.0021 (11)	−0.0018 (12)
C7	0.0500 (12)	0.0441 (11)	0.0668 (13)	−0.0064 (9)	0.0014 (10)	0.0067 (10)
C8	0.0421 (10)	0.0300 (9)	0.0465 (10)	0.0025 (7)	0.0077 (8)	−0.0030 (7)
C9	0.0420 (10)	0.0341 (10)	0.0526 (11)	−0.0001 (8)	0.0062 (8)	0.0035 (8)
C10	0.0384 (10)	0.0367 (10)	0.0566 (11)	0.0008 (8)	0.0071 (8)	−0.0052 (8)
C11	0.0433 (10)	0.0433 (10)	0.0466 (10)	0.0094 (8)	0.0056 (8)	−0.0033 (8)
C12	0.0537 (12)	0.0437 (11)	0.0518 (11)	0.0047 (9)	0.0121 (9)	0.0070 (9)
C13	0.0468 (11)	0.0339 (10)	0.0550 (11)	−0.0028 (8)	0.0106 (9)	−0.0001 (8)
N1	0.0454 (9)	0.0276 (7)	0.0529 (9)	−0.0039 (6)	0.0008 (7)	−0.0025 (6)
O1	0.0621 (9)	0.0302 (7)	0.0630 (8)	−0.0058 (6)	−0.0065 (7)	0.0000 (6)
Cl1	0.0441 (3)	0.0544 (3)	0.0815 (4)	−0.0097 (2)	−0.0030 (2)	0.0019 (3)
Cl2	0.0620 (4)	0.0785 (4)	0.0540 (3)	0.0084 (3)	−0.0070 (2)	−0.0007 (3)

Geometric parameters (Å, °)

C1—O1	1.225 (2)	C8—C9	1.388 (2)
C1—N1	1.356 (2)	C8—C13	1.388 (3)
C1—C2	1.491 (2)	C8—N1	1.409 (2)
C2—C3	1.378 (3)	C9—C10	1.385 (3)
C2—C7	1.387 (3)	C9—H9	0.93
C3—C4	1.379 (3)	C10—C11	1.384 (3)
C3—H3	0.93	C10—Cl1	1.7293 (18)
C4—C5	1.358 (3)	C11—C12	1.387 (3)
C4—H4	0.93	C11—Cl2	1.7228 (19)
C5—C6	1.375 (3)	C12—C13	1.371 (3)
C5—H5	0.93	C12—H12	0.93
C6—C7	1.377 (3)	C13—H13	0.93
C6—H6	0.93	N1—H1	0.86
C7—H7	0.93		
O1—C1—N1	122.29 (16)	C9—C8—C13	119.44 (16)
O1—C1—C2	121.63 (16)	C9—C8—N1	122.58 (16)
N1—C1—C2	116.07 (14)	C13—C8—N1	117.97 (16)
C3—C2—C7	118.71 (17)	C10—C9—C8	119.65 (17)
C3—C2—C1	118.64 (16)	C10—C9—H9	120.2
C7—C2—C1	122.51 (16)	C8—C9—H9	120.2
C2—C3—C4	120.44 (19)	C11—C10—C9	120.79 (17)
C2—C3—H3	119.8	C11—C10—Cl1	120.56 (15)
C4—C3—H3	119.8	C9—C10—Cl1	118.63 (14)

C5—C4—C3	120.6 (2)	C10—C11—C12	118.98 (17)
C5—C4—H4	119.7	C10—C11—Cl2	121.52 (15)
C3—C4—H4	119.7	C12—C11—Cl2	119.50 (15)
C4—C5—C6	119.8 (2)	C13—C12—C11	120.59 (18)
C4—C5—H5	120.1	C13—C12—H12	119.7
C6—C5—H5	120.1	C11—C12—H12	119.7
C5—C6—C7	120.3 (2)	C12—C13—C8	120.48 (17)
C5—C6—H6	119.9	C12—C13—H13	119.8
C7—C6—H6	119.9	C8—C13—H13	119.8
C6—C7—C2	120.2 (2)	C1—N1—C8	126.38 (14)
C6—C7—H7	119.9	C1—N1—H1	116.8
C2—C7—H7	119.9	C8—N1—H1	116.8
O1—C1—C2—C3	28.3 (3)	C8—C9—C10—Cl1	177.27 (14)
N1—C1—C2—C3	−153.17 (17)	C9—C10—C11—C12	2.7 (3)
O1—C1—C2—C7	−147.4 (2)	Cl1—C10—C11—C12	−175.68 (14)
N1—C1—C2—C7	31.1 (3)	C9—C10—C11—Cl2	−177.98 (14)
C7—C2—C3—C4	−0.4 (3)	Cl1—C10—C11—Cl2	3.6 (2)
C1—C2—C3—C4	−176.28 (18)	C10—C11—C12—C13	−1.9 (3)
C2—C3—C4—C5	0.3 (3)	Cl2—C11—C12—C13	178.72 (15)
C3—C4—C5—C6	0.4 (4)	C11—C12—C13—C8	−0.4 (3)
C4—C5—C6—C7	−0.9 (4)	C9—C8—C13—C12	1.9 (3)
C5—C6—C7—C2	0.8 (3)	N1—C8—C13—C12	−179.20 (17)
C3—C2—C7—C6	−0.1 (3)	O1—C1—N1—C8	8.0 (3)
C1—C2—C7—C6	175.59 (19)	C2—C1—N1—C8	−170.51 (16)
C13—C8—C9—C10	−1.2 (3)	C9—C8—N1—C1	−37.6 (3)
N1—C8—C9—C10	−179.99 (16)	C13—C8—N1—C1	143.61 (18)
C8—C9—C10—C11	−1.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.16	2.9568 (19)	153

Symmetry codes: (i) *x*, *y*−1, *z*.

Fig. 1

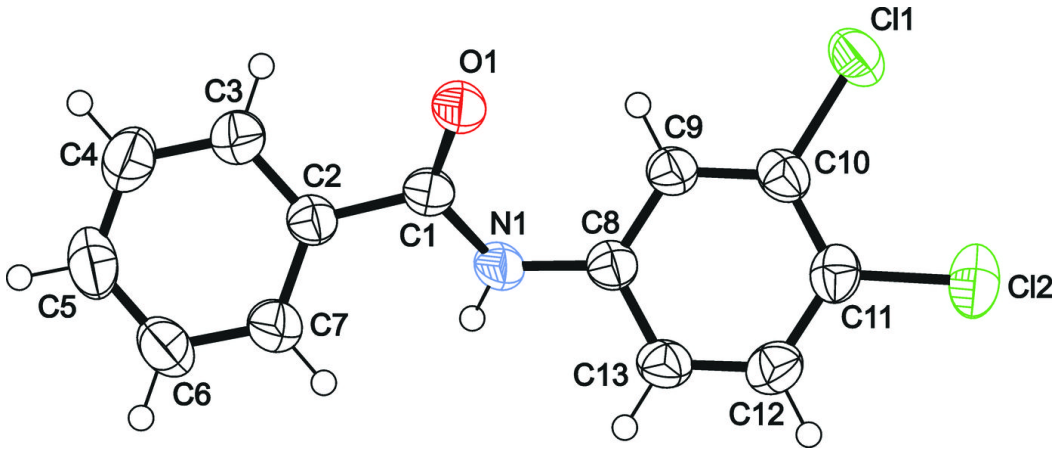

Fig. 2