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N-(2,3-Dichlorophenyl)benzamide

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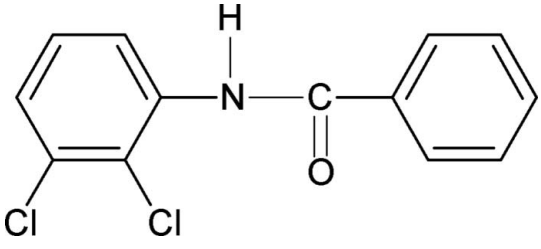
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.005 Å; R factor = 0.036; wR factor = 0.093; data-to-parameter ratio = 15.1.

In the structure of the title compound, $C_{13}H_9Cl_2NO$, the conformation of the N—H bond is *syn* to the chloro substituents on the aniline benzene ring, similar to that observed in *N*-(2,3-dichlorophenyl)acetamide, but in contrast to the anti conformation observed with respect to the *ortho*-Cl substituent in *N*-(2-chlorophenyl)benzamide. The structure closely resembles the structures of 2-chloro-*N*-phenylbenzamide, *N*-(2-chlorophenyl)benzamide and *N*-(2,3-dichlorophenyl)acetamide. The molecules are linked into a chain through an N—H···O hydrogen bond.

Related literature

For related literature, see: Gowda *et al.* (2003); Gowda, Foro *et al.* (2007); Gowda, Kozisek *et al.* (2007); Gowda, Sowmya *et al.* (2007).



Experimental

Crystal data

$C_{13}H_9Cl_2NO$
M_r = 266.11
Orthorhombic, *Pbcn*
a = 24.2968 (12) Å
b = 11.3273 (5) Å
c = 8.7396 (3) Å
V = 2405.29 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 295 (2) K
0.45 × 0.09 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.894, T_{max} = 0.961
21027 measured reflections
2319 independent reflections
981 reflections with $I > 2\sigma(I)$
R_{int} = 0.097

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 0.91
2319 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1^{i}	0.86	2.17	2.952 (3)	152
N1—H1*N*···Cl1	0.86	2.57	2.929 (3)	106
C9—H9···O1	0.93	2.34	2.861 (4)	115

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

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: BT2404).

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supplementary materials

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N-(2,3-Dichlorophenyl)benzamide

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Comment

In the present work, the structure of *N*-(2,3-dichlorophenyl)-benzamide has been determined to explore the substituent effects on the structures of N-aromatic amides (Gowda *et al.*, 2003; Gowda, Foro, & Fuess, 2007; Gowda, Kozisek, *et al.*, 2007; Gowda, Sowmya, *et al.*, 2007). The conformation of the N—H bond (Fig. 1) is *syn* to the chloro substituents in the aniline phenyl ring, similar to that observed in *N*-(2,3-dichlorophenyl)-acetamide (Gowda, Foro, & Fuess, 2007), but in contrast to the anti conformation observed with respect to the *ortho*-Cl substituent in *N*-(2-chlorophenyl)-benzamide (Gowda, Sowmya, *et al.*, 2007). The structure resembles the structure of *N*-(phenyl)-2-chlorobenzamide (Gowda *et al.*, 2003), *N*-(2-chlorophenyl)-benzamide (Gowda, Sowmya, *et al.*, 2007) and *N*-(2,3-dichlorophenyl)-acetamide (Gowda, Foro, & Fuess, 2007). The packing diagram showis the infinite chain of molecules along [0 0 1] linked by N—H···O hydrogen bonds (Fig. 2 and Table 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.

Refinement

H atoms were found in a difference map and refined using a riding model with C—H distances of 0.93Å and 0.86Å for the H—N distance and with U_{iso}(H) = 1.2 U_{eq}(C,*N*).

Figures

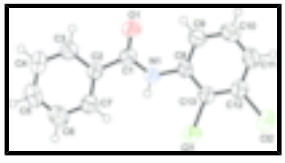

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

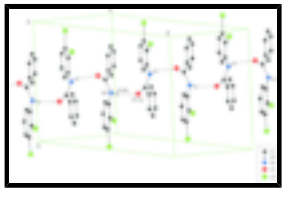

Fig. 2. Part of crystal structure of the title compound showing the infinite chain of molecules along [0 0 1] linked by hydrogen bonds N1—H1N···O1(i). Symmetry operation (i): x, $-y+1$, $z+1/2$.

N-(2,3-Dichlorophenyl)benzamide

Crystal data

$C_{13}H_9Cl_2NO$	F_{000} = 1088
M_r = 266.11	D_x = 1.47 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 2616 reflections
a = 24.2968 (12) Å	θ = 3.1–29.4º
b = 11.3273 (5) Å	μ = 0.52 mm^{-1}
c = 8.7396 (3) Å	*T* = 295 (2) K
V = 2405.29 (18) Å^3	Needle, colorless
Z = 8	0.45 × 0.09 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur diffractometer	981 reflections with $I > 2\sigma(I)$
Radiation source: Enhance (Mo) X-ray Source	R_{int} = 0.097
Monochromator: graphite	θ_{max} = 25.9º
φ scans, and ω scans with κ offsets	θ_{min} = 4.3º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)	*h* = −29→29
T_{min} = 0.894, T_{max} = 0.961	*k* = −13→13
21027 measured reflections	*l* = −10→10
2319 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$(\Delta/\sigma)_{max}$ = 0.002
$wR(F^2)$ = 0.093	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
S = 0.91	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
2319 reflections	Extinction correction: none
154 parameters	

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.37448 (11)	0.4513 (3)	0.2398 (3)	0.0476 (7)
C2	0.33837 (11)	0.3829 (3)	0.3452 (3)	0.0444 (7)
C3	0.34131 (12)	0.2616 (3)	0.3412 (3)	0.0555 (8)
H3	0.3652	0.2249	0.2730	0.067*
C4	0.30922 (14)	0.1938 (3)	0.4369 (4)	0.0676 (9)
H4	0.3122	0.1120	0.4358	0.081*
C5	0.27301 (13)	0.2478 (4)	0.5336 (4)	0.0709 (10)
H5	0.2513	0.2023	0.5986	0.085*
C6	0.26823 (13)	0.3682 (4)	0.5359 (4)	0.0712 (10)
H6	0.2429	0.4040	0.6009	0.085*
C7	0.30086 (12)	0.4365 (3)	0.4420 (3)	0.0562 (8)
H7	0.2977	0.5183	0.4437	0.067*
C8	0.41571 (11)	0.6480 (3)	0.1992 (3)	0.0422 (7)
C9	0.45461 (12)	0.6195 (3)	0.0898 (3)	0.0559 (8)
H9	0.4629	0.5408	0.0700	0.067*
C10	0.48119 (12)	0.7080 (3)	0.0099 (3)	0.0632 (9)
H10	0.5071	0.6881	−0.0641	0.076*
C11	0.47010 (12)	0.8235 (3)	0.0375 (4)	0.0646 (9)
H11	0.4883	0.8820	−0.0174	0.078*
C12	0.43170 (13)	0.8539 (3)	0.1474 (3)	0.0560 (8)
C13	0.40443 (11)	0.7666 (3)	0.2283 (3)	0.0477 (8)
N1	0.38766 (9)	0.5620 (2)	0.2842 (2)	0.0491 (6)
H1N	0.3777	0.5821	0.3750	0.059*
O1	0.39099 (8)	0.40812 (18)	0.1197 (2)	0.0641 (6)
Cl1	0.35585 (4)	0.80396 (7)	0.36269 (8)	0.0689 (3)
Cl2	0.41772 (4)	1.00012 (8)	0.18131 (11)	0.0968 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0566 (19)	0.043 (2)	0.0428 (17)	0.0072 (16)	−0.0068 (15)	−0.0002 (16)
C2	0.0485 (19)	0.045 (2)	0.0400 (15)	−0.0013 (15)	−0.0039 (14)	−0.0011 (16)
C3	0.060 (2)	0.055 (2)	0.0521 (17)	0.0006 (16)	−0.0035 (17)	−0.0026 (17)
C4	0.071 (2)	0.054 (2)	0.077 (2)	−0.014 (2)	−0.012 (2)	0.012 (2)
C5	0.056 (2)	0.090 (3)	0.066 (2)	−0.022 (2)	−0.0032 (19)	0.018 (2)
C6	0.058 (2)	0.083 (3)	0.072 (2)	−0.011 (2)	0.0035 (18)	−0.004 (2)
C7	0.057 (2)	0.054 (2)	0.0570 (18)	−0.0028 (18)	−0.0022 (17)	−0.0011 (18)
C8	0.0471 (18)	0.044 (2)	0.0357 (15)	0.0009 (15)	−0.0022 (13)	0.0061 (14)
C9	0.0564 (19)	0.059 (2)	0.0526 (17)	0.0070 (17)	0.0064 (16)	0.0028 (17)
C10	0.050 (2)	0.077 (3)	0.0624 (19)	0.0063 (19)	0.0122 (16)	0.003 (2)
C11	0.055 (2)	0.063 (3)	0.075 (2)	−0.0085 (19)	0.0081 (18)	0.0079 (19)
C12	0.060 (2)	0.051 (2)	0.0569 (18)	−0.0016 (16)	−0.0002 (17)	0.0035 (17)
C13	0.0522 (19)	0.051 (2)	0.0402 (15)	−0.0011 (16)	−0.0025 (14)	0.0012 (15)
N1	0.0679 (16)	0.0411 (16)	0.0383 (12)	0.0027 (14)	0.0059 (11)	−0.0020 (13)

O1	0.0942 (16)	0.0539 (14)	0.0442 (11)	0.0014 (12)	0.0097 (11)	−0.0086 (10)
Cl1	0.0925 (6)	0.0530 (5)	0.0613 (5)	0.0056 (5)	0.0242 (4)	−0.0040 (4)
Cl2	0.1238 (8)	0.0477 (6)	0.1188 (8)	−0.0073 (5)	0.0328 (6)	0.0059 (5)

Geometric parameters (Å, °)

C1—O1	1.226 (3)	C8—C9	1.383 (4)
C1—N1	1.351 (3)	C8—C13	1.395 (4)
C1—C2	1.490 (4)	C8—N1	1.401 (3)
C2—C3	1.377 (4)	C9—C10	1.382 (4)
C2—C7	1.384 (4)	C9—H9	0.9300
C3—C4	1.377 (4)	C10—C11	1.357 (4)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.364 (4)	C11—C12	1.383 (4)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.369 (5)	C12—C13	1.384 (4)
C5—H5	0.9300	C12—Cl2	1.716 (3)
C6—C7	1.378 (4)	C13—Cl1	1.718 (3)
C6—H6	0.9300	N1—H1N	0.8600
C7—H7	0.9300		
O1—C1—N1	122.6 (3)	C9—C8—C13	119.0 (3)
O1—C1—C2	120.9 (3)	C9—C8—N1	122.5 (3)
N1—C1—C2	116.4 (2)	C13—C8—N1	118.5 (2)
C3—C2—C7	119.2 (3)	C10—C9—C8	120.0 (3)
C3—C2—C1	118.3 (3)	C10—C9—H9	120.0
C7—C2—C1	122.5 (3)	C8—C9—H9	120.0
C2—C3—C4	120.7 (3)	C11—C10—C9	121.1 (3)
C2—C3—H3	119.6	C11—C10—H10	119.4
C4—C3—H3	119.6	C9—C10—H10	119.4
C5—C4—C3	119.4 (3)	C10—C11—C12	119.9 (3)
C5—C4—H4	120.3	C10—C11—H11	120.1
C3—C4—H4	120.3	C12—C11—H11	120.1
C4—C5—C6	120.7 (3)	C11—C12—C13	119.9 (3)
C4—C5—H5	119.7	C11—C12—Cl2	119.6 (3)
C6—C5—H5	119.7	C13—C12—Cl2	120.4 (2)
C5—C6—C7	120.1 (3)	C12—C13—C8	120.1 (2)
C5—C6—H6	120.0	C12—C13—Cl1	120.1 (2)
C7—C6—H6	120.0	C8—C13—Cl1	119.8 (2)
C6—C7—C2	119.8 (3)	C1—N1—C8	127.4 (2)
C6—C7—H7	120.1	C1—N1—H1N	116.3
C2—C7—H7	120.1	C8—N1—H1N	116.3
O1—C1—C2—C3	25.7 (4)	C9—C10—C11—C12	0.1 (5)
N1—C1—C2—C3	−154.3 (2)	C10—C11—C12—C13	−0.4 (4)
O1—C1—C2—C7	−151.9 (3)	C10—C11—C12—Cl2	−179.8 (2)
N1—C1—C2—C7	28.1 (4)	C11—C12—C13—C8	0.1 (4)
C7—C2—C3—C4	−2.9 (4)	Cl2—C12—C13—C8	179.5 (2)
C1—C2—C3—C4	179.4 (2)	C11—C12—C13—Cl1	−178.9 (2)
C2—C3—C4—C5	1.9 (4)	Cl2—C12—C13—Cl1	0.5 (3)
C3—C4—C5—C6	0.2 (5)	C9—C8—C13—C12	0.4 (4)

C4—C5—C6—C7	−1.2 (5)	N1—C8—C13—C12	179.5 (2)
C5—C6—C7—C2	0.1 (4)	C9—C8—C13—Cl1	179.48 (19)
C3—C2—C7—C6	1.9 (4)	N1—C8—C13—Cl1	−1.5 (3)
C1—C2—C7—C6	179.4 (3)	O1—C1—N1—C8	7.4 (4)
C13—C8—C9—C10	−0.7 (4)	C2—C1—N1—C8	−172.6 (2)
N1—C8—C9—C10	−179.7 (3)	C9—C8—N1—C1	−30.1 (4)
C8—C9—C10—C11	0.5 (4)	C13—C8—N1—C1	150.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···O1^{i}	0.86	2.17	2.952 (3)	152
N1—H1N···Cl1	0.86	2.57	2.929 (3)	106
C9—H9···O1	0.93	2.34	2.861 (4)	115

Symmetry codes: (i) *x*, −*y*+1, *z*+1/2.

Fig. 1

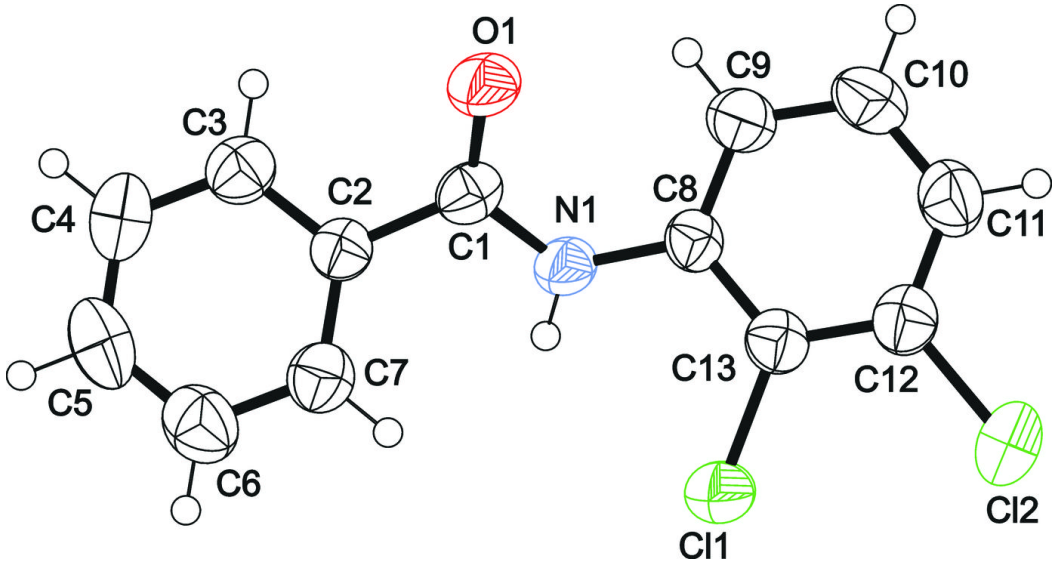

Fig. 2