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N-(2,4-Dichlorophenyl)acetamide

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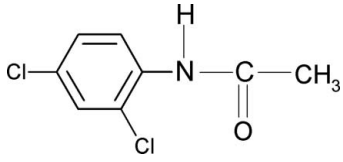
Key indicators: single-crystal X-ray study; T = 302 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.105; data-to-parameter ratio = 15.2.

The crystal system, unit-cell dimensions and space group of the title compound, $C_8H_7Cl_2NO$, have already been reported [Ananthamurthy & Murthy (1973). *Z. Kristallogr.* **137**, 320]. The bond parameters are similar to those in *N*-(2-chlorophenyl)acetamide and *N*-(2,3-dichlorophenyl)acetamide. The N—H bond is *syn* to the *ortho*-chloro substituent. The molecules are linked into chains through N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2007*a*,*b*); Gowda, Svoboda *et al.* (2007); Pies *et al.* (1971); Shilpa & Gowda (2007); Clark & Reid (1995); Gowda, Kozisek *et al.* (2007).



Experimental

Crystal data

$C_8H_7Cl_2NO$
M_r = 204.05
Monoclinic, $P2_1/c$
a = 8.0552 (5) Å
b = 11.773 (1) Å
c = 9.7286 (5) Å
β = 102.547 (6)°
V = 900.57 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 302 (2) K
0.60 × 0.30 × 0.30 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.690, T_{max} = 0.825
13123 measured reflections
1836 independent reflections
1451 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.105
S = 1.08
1836 reflections
121 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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}	0.83 (3)	2.14 (3)	2.956 (2)	171 (2)

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

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: *PLATON* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2403).

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supplementary materials

Acta Cryst. (2007). E**63**, o3308 [**doi:10.1107/S1600536807030292**]

N-(2,4-Dichlorophenyl)acetamide

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Comment

The structure of *N*-(2,4-dichlorophenyl)-acetamide has been determined as part of a study on the systematization of the crystal structures of N-aromatic amides (Gowda *et al.*, 2007*a*, *b*; Gowda, Kozisek *et al.*, 2007; Gowda, Svoboda *et al.*, 2007). The N—H bond is *syn* to the *ortho*-chloro substituent (Fig. 1), similar to that observed in *N*-(2-chlorophenyl)-acetamide (Gowda, Svoboda *et al.*, 2007) and *N*-(2,3-dichlorophenyl)-acetamide (Gowda *et al.*, 2007*b*). The crystal system, unit-cell dimensions (a = 8.27 (02) Å, b= 11.94 (02) Å, c = 9.89 (02) Å; β = 103.20°, at 283–303 K) and the space group of the title compound have already been reported (Ananthamurthy & Murthy, 1973). The geometric parameters are similar to those of other acetanilides (Gowda *et al.*, 2007*a*, *b*; Gowda, Svoboda *et al.*, 2007; Gowda, Kozisek *et al.*, 2007). The molecules are linked into chains through N—H···O hydrogen bonds (Fig. 2 & Table 1).

Experimental

The title compound was prepared according to the literature method of Shilpa & Gowda (2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared, NMR (Shilpa & Gowda, 2007) and NQR spectra (Pies *et al.*, 1971). Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution (2 g in about 30 ml e thanol).

Refinement

The H atoms were located in difference map and their positions (except the methyl group) were refined, with U_{iso}(H) = 1.2 U_{eq}(C,*N*).

Figures

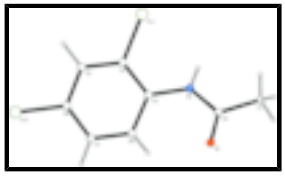

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

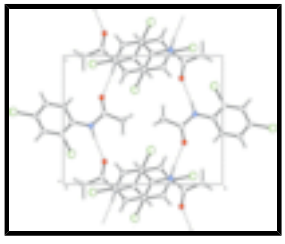

Fig. 2. Hydrogen bonding in the title compound. Hydrogen bonds are shown as dashed lines.

N-(2,4-Dichlorophenyl)acetamide

Crystal data

$C_8H_7Cl_2NO$	F_{000} = 416
M_r = 204.05	D_x = 1.505 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P2ybc	Cell parameters from 5521 reflections
a = 8.0552 (5) Å	θ = 2.2–25.3º
b = 11.773 (1) Å	μ = 0.67 mm^{-1}
c = 9.7286 (5) Å	T = 302 (2) K
β = 102.547 (6)º	Rod shape, colourless
V = 900.57 (11) Å^3	0.60 × 0.30 × 0.30 mm
Z = 4	

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector	1836 independent reflections
Radiation source: Enhance (Mo) X-ray Source	1451 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.017
Detector resolution: 8.4012 pixels mm^{-1}	θ_{max} = 26.4º
T = 302(2) K	θ_{min} = 2.6º
Rotation method data acquisition using ω and φ scans	h = −10→10
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2006)	k = −14→14
T_{min} = 0.690, T_{max} = 0.825	l = −12→12
13123 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.105	$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.5653P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
1836 reflections	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
121 parameters	$\Delta\rho_{min}$ = −0.31 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	0.3264 (4)	0.3736 (2)	0.4935 (3)	0.0608 (7)
H1A	0.4447	0.3939	0.5148	0.073*
H1B	0.2635	0.4277	0.5358	0.073*
H1C	0.2844	0.3735	0.3933	0.073*
C2	0.3057 (3)	0.25823 (18)	0.5505 (2)	0.0437 (5)
C3	0.2610 (3)	0.05800 (17)	0.4836 (2)	0.0385 (4)
C4	0.1505 (3)	−0.00918 (19)	0.3886 (2)	0.0404 (5)
C5	0.1311 (3)	−0.1240 (2)	0.4114 (2)	0.0484 (5)
H5	0.048 (3)	−0.170 (2)	0.345 (3)	0.058*
C6	0.2257 (3)	−0.17142 (19)	0.5320 (2)	0.0521 (6)
C7	0.3370 (3)	−0.1079 (2)	0.6283 (2)	0.0528 (6)
H7	0.408 (3)	−0.140 (2)	0.707 (3)	0.063*
C8	0.3550 (3)	0.0062 (2)	0.6041 (2)	0.0466 (5)
H8	0.432 (3)	0.049 (2)	0.663 (3)	0.056*
N1	0.2801 (2)	0.17373 (15)	0.45465 (18)	0.0424 (4)
H1	0.280 (3)	0.192 (2)	0.373 (3)	0.051*
O1	0.3106 (3)	0.24142 (14)	0.67523 (16)	0.0616 (5)
Cl1	0.03170 (8)	0.05085 (5)	0.23606 (6)	0.0570 (2)
Cl2	0.19964 (13)	−0.31485 (6)	0.56382 (8)	0.0838 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0893 (19)	0.0441 (13)	0.0472 (13)	−0.0051 (12)	0.0110 (12)	−0.0007 (11)
C2	0.0544 (13)	0.0423 (11)	0.0332 (11)	−0.0009 (10)	0.0069 (9)	−0.0038 (9)
C3	0.0459 (11)	0.0406 (11)	0.0313 (10)	0.0027 (8)	0.0132 (8)	−0.0032 (8)
C4	0.0457 (11)	0.0455 (11)	0.0309 (10)	0.0024 (9)	0.0103 (8)	−0.0010 (8)
C5	0.0596 (14)	0.0475 (12)	0.0394 (11)	−0.0071 (11)	0.0138 (10)	−0.0057 (10)
C6	0.0734 (16)	0.0385 (11)	0.0475 (13)	0.0009 (11)	0.0202 (11)	0.0015 (10)
C7	0.0676 (15)	0.0492 (13)	0.0401 (12)	0.0083 (11)	0.0087 (11)	0.0061 (10)
C8	0.0535 (13)	0.0470 (12)	0.0371 (11)	−0.0008 (10)	0.0047 (9)	−0.0023 (9)
N1	0.0608 (11)	0.0399 (9)	0.0266 (8)	−0.0013 (8)	0.0098 (8)	−0.0002 (7)

O1	0.1027 (14)	0.0501 (10)	0.0318 (8)	−0.0003 (9)	0.0142 (8)	−0.0059 (7)
Cl1	0.0643 (4)	0.0580 (4)	0.0415 (3)	−0.0014 (3)	−0.0043 (2)	0.0008 (2)
Cl2	0.1339 (7)	0.0443 (4)	0.0703 (5)	−0.0095 (4)	0.0153 (4)	0.0081 (3)

Geometric parameters (Å, °)

C1—C2	1.490 (3)	C4—Cl1	1.732 (2)
C1—H1A	0.9600	C5—C6	1.372 (3)
C1—H1B	0.9600	C5—H5	0.99 (3)
C1—H1C	0.9600	C6—C7	1.369 (3)
C2—O1	1.222 (3)	C6—Cl2	1.738 (2)
C2—N1	1.348 (3)	C7—C8	1.377 (3)
C3—C4	1.384 (3)	C7—H7	0.93 (3)
C3—C8	1.391 (3)	C8—H8	0.90 (3)
C3—N1	1.406 (3)	N1—H1	0.83 (3)
C4—C5	1.384 (3)		
C2—C1—H1A	109.5	C6—C5—C4	118.3 (2)
C2—C1—H1B	109.5	C6—C5—H5	120.5 (15)
H1A—C1—H1B	109.5	C4—C5—H5	121.2 (15)
C2—C1—H1C	109.5	C7—C6—C5	121.5 (2)
H1A—C1—H1C	109.5	C7—C6—Cl2	119.70 (19)
H1B—C1—H1C	109.5	C5—C6—Cl2	118.80 (19)
O1—C2—N1	122.3 (2)	C6—C7—C8	119.6 (2)
O1—C2—C1	122.4 (2)	C6—C7—H7	122.2 (17)
N1—C2—C1	115.35 (18)	C8—C7—H7	118.0 (17)
C4—C3—C8	117.8 (2)	C7—C8—C3	120.9 (2)
C4—C3—N1	120.17 (18)	C7—C8—H8	121.8 (16)
C8—C3—N1	122.00 (19)	C3—C8—H8	117.3 (16)
C3—C4—C5	122.0 (2)	C2—N1—C3	125.70 (17)
C3—C4—Cl1	119.64 (17)	C2—N1—H1	116.4 (17)
C5—C4—Cl1	118.37 (17)	C3—N1—H1	117.9 (17)
C8—C3—C4—C5	0.6 (3)	Cl2—C6—C7—C8	−178.80 (19)
N1—C3—C4—C5	178.39 (19)	C6—C7—C8—C3	0.4 (4)
C8—C3—C4—Cl1	−179.47 (16)	C4—C3—C8—C7	−0.6 (3)
N1—C3—C4—Cl1	−1.7 (3)	N1—C3—C8—C7	−178.4 (2)
C3—C4—C5—C6	−0.2 (3)	O1—C2—N1—C3	−2.0 (4)
Cl1—C4—C5—C6	179.82 (18)	C1—C2—N1—C3	178.5 (2)
C4—C5—C6—C7	−0.1 (4)	C4—C3—N1—C2	144.3 (2)
C4—C5—C6—Cl2	178.75 (17)	C8—C3—N1—C2	−38.0 (3)
C5—C6—C7—C8	0.0 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.83 (3)	2.14 (3)	2.956 (2)	171 (2)

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

Fig. 1

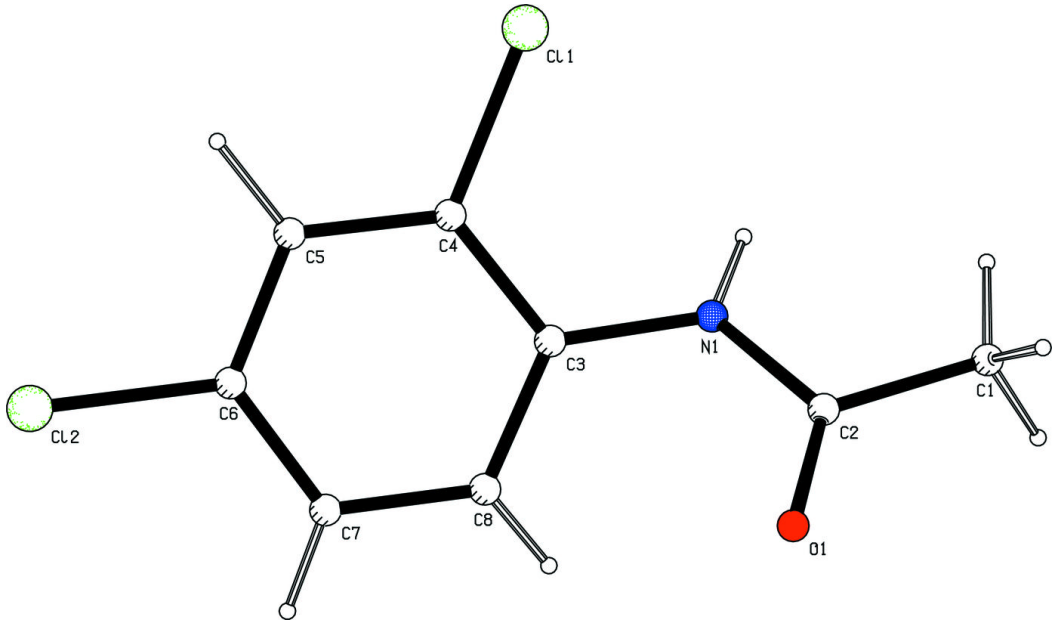

Fig. 2