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N-(2,3-Dichlorophenyl)acetamide

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Key indicators
Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.102
Data-to-parameter ratio = 13.8

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

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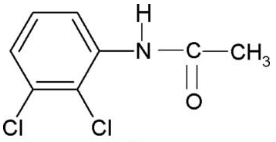
The conformation of the N—H bond in the structure of the title compound (23DCPA), $C_8H_7Cl_2NO$, is *syn* to either the *ortho* or *meta* chloro substituent. The geometric parameters of 23DCPA are similar to related amides. The amide H atom is simultaneously involved in an intramolecular hydrogen bond with the *ortho* Cl atom and an intermolecular hydrogen bond with the O atom of the carbonyl group.

Comment

Amides are of interest as conjugation between the nitrogen lone-pair electrons and the carbonyl π-bond results in distinct physical and chemical properties. The amide unit is also an important constituent of many biologically relevant compounds. Thus structural studies of amides are of interest (Gowda *et al.*, 2006, 2007, 2007*a*,*b*; Jones *et al.*, 1990; Wan *et al.*, 2006). As a part of a study of the effect of ring and side-chain substitutions on the solid-state geometry of this class of compounds, we report here the crystal structure of *N*-(2,3-dichlorophenyl)acetamide (23DCPA), (I).



(I)

The title compound crystallizes with the *meta* Cl substituent showing a *syn* conformation with respect to the N—H bond. This is in contrast to the *anti* conformation observed for *N*-(3,4-dichlorophenyl)acetamide (Jones *et al.*, 1990). The relatively large bond angle of 125.9 (3)° for C2—N—C5 may be due to steric interaction between the O atom and H10. The corresponding torsion angles are 145.3 (3) and −36.0 (5)° for C2—N4—C5—C6 and C2—N4—C5—C10, respectively. The amide H atom is simultaneously involved in an intramolecular hydrogen bond with the *ortho* Cl atom and an intermolecular hydrogen bond with the O atom of the carbonyl group (Table 1 and Fig. 2). The intramolecular hydrogen bond observed in 23DCPA, involving the *ortho* Cl atom as the acceptor site, is similar to the weak hydrogen bonds observed in the crystal structures of similar compounds.

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 by slow evaporation of an ethanol solution (2 g in about 30 ml ethanol) and used for X-ray diffraction studies at room temperature.

Crystal data

$C_8H_7Cl_2NO$
$M_r = 204.05$
Monoclinic, $P2_1/c$
$a = 4.7524$ (5) Å
$b = 12.246$ (1) Å
$c = 15.140$ (1) Å
$\beta = 98.915$ (7)°
$V = 870.5$ (1) Å^3
$Z = 4$
Cu $K\alpha$ radiation
$\mu = 6.29$ mm^{-1}
$T = 299$ (2) K
0.28 × 0.06 × 0.04 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.485$, $T_{\max} = 0.627$ (expected range = 0.601–0.778)
1923 measured reflections
1560 independent reflections
1072 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
3 standard reflections
frequency: 120 min
intensity decay: 4.3%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.102$
$S = 1.06$
1560 reflections
113 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.27$ 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
N4—H4N···Cl11	0.850 (10)	2.63 (3)	2.949 (3)	104 (2)
N4—H4N···O3$^{\rm i}$	0.850 (10)	2.14 (2)	2.896 (4)	148 (3)

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

All H atoms attached to C atoms were positioned geometrically and treated as riding, with C—H = 0.93 (CH aromatic) or 0.96 Å (CH_3) and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(CH_3). The H atom attached to N4 was found in a difference map and refined with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(N).

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); 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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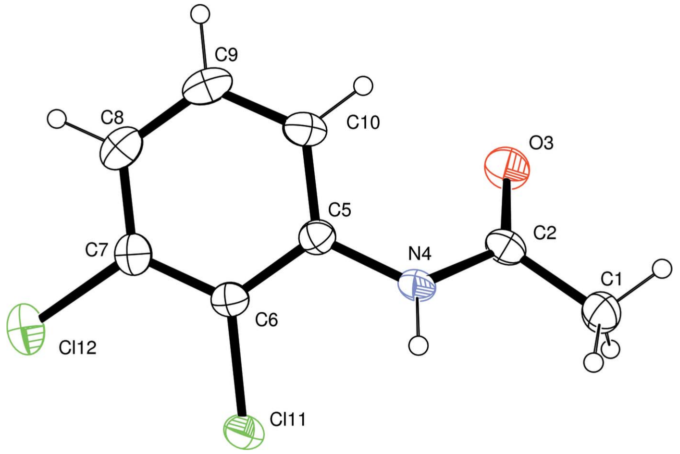

Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

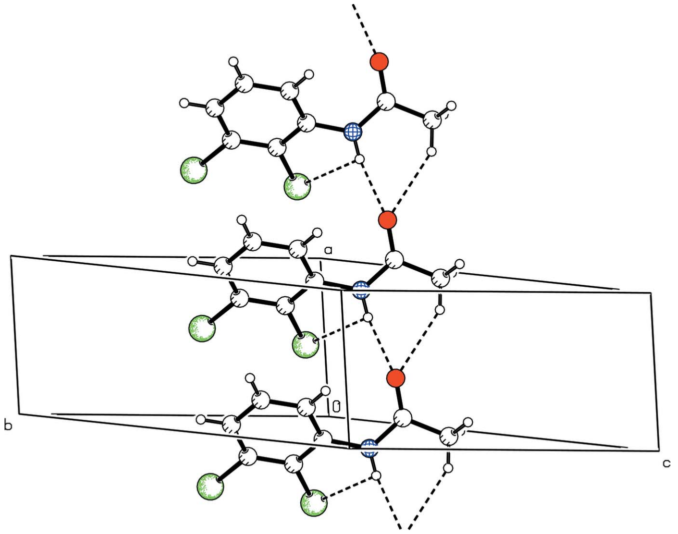

Figure 2
Typical hydrogen-bond (dashed lines) bridges observed in the title compound.

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