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N-(3,5-Dichlorophenyl)acetamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.011 Å
R factor = 0.055
wR factor = 0.152
Data-to-parameter ratio = 8.6

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

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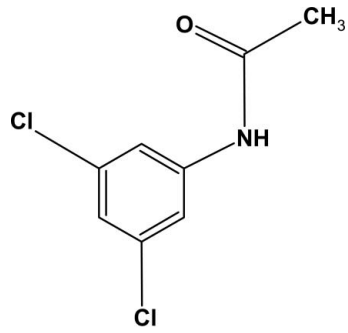
In the title compound, $C_8H_7Cl_2NO$, all bond lengths and angles are normal. The molecular skeleton is essentially planar. The intermolecular N—H···O hydrogen bonds link the molecules into zigzag chains running along the *a* axis.

Comment

In continuation of a structural study of substituted amides (Gowda *et al.*, 2006, 2007), we report here the crystal structure of *N*-(3,5-dichlorophenyl)-acetamide (35DCPA) (Fig. 1).



(I)

The bond lengths and angles in 35DCPA show normal values (Allen *et al.*, 1987). The molecular skeleton is essentially planar, the maximum deviations from the mean plane being 0.057 (8) Å for atom C1 and −0.035 (8) Å for O3. Symmetric substitutions such as di-*meta* or di-*ortho* substitutions (Nagarajan *et al.*, 1986) of electron-withdrawing groups in the parent amide, *N*-(phenyl)-acetamide (Brown & Corbridge, 1954; Brown, 1966), do not alter the conformation.

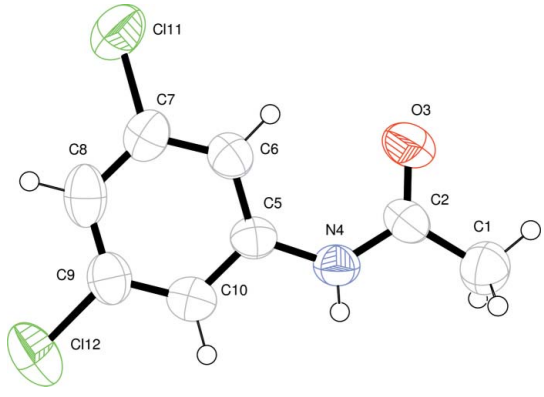


Figure 1
The molecular structure of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 40% probability level.

However, di-*meta* substitution of Cl atoms significantly alters the C6-C5-C10 angle from 121.2 to 119.0 (7)°, while other geometrical parameters are marginally affected.

Intermolecular N—H···O hydrogen bonds (Table 1) link the molecules into zigzag chains running along the *a* axis (Fig. 2). The C9···C10^{ii} short contact of 3.57 (1) Å indicates the presence of π–π stacking interactions, which contribute to the crystal packing stability [symmetry code: (ii) x, y, $1 + z$].

Experimental

The title compound was prepared according to the literature method (Pies *et al.*, 1971). It was characterized by recording its infrared, NMR and NQR spectra (Pies *et al.*, 1971; Shilpa & Gowda, 2007). Single crystals were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_8H_7Cl_2NO$
M_r = 204.05
Orthorhombic, $Pna2_1$
a = 9.5670 (10) Å
b = 24.116 (5) Å
c = 3.9552 (6) Å
V = 912.5 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 6.00 mm^{-1}
T = 299 (2) K
0.57 × 0.04 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.945, T_{max} = 0.996
(expected range = 0.792–0.835)
959 measured reflections
943 independent reflections
541 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
3 standard reflections
frequency: 120 min
intensity decay: 2.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.152
S = 1.04
943 reflections
110 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter: 0.03 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4*N*···O3^{i}	0.86	1.98	2.808 (7)	163

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

All H atoms were positioned geometrically, with C—H = 0.93 Å (CH aromatic) or 0.96 Å (CH_3), N—H = 0.86 Å, and treated as riding with U_{iso}(H) = 1.2U_{eq}(CH or NH) and U_{iso}(H) = 1.5U_{eq}(CH_3).

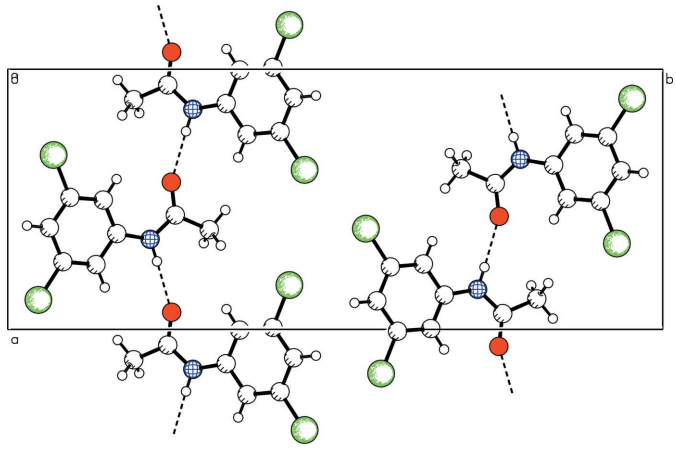


Figure 2
A portion of the crystal packing, viewed down the *c* axis. Dashed lines denote hydrogen bonds.

Data collection: *CAD-4-PC* (Nonius, 1996); cell refinement: Nonius *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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