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2,2,2-Trichloro-*N*-(3,4-dichlorophenyl)acetamide

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.028
wR factor = 0.067
Data-to-parameter ratio = 14.1

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

In the title compound, $C_8H_4Cl_5NO$, the N—H bond is *anti* to the *meta*-Cl substituent, similar to the chain-unsubstituted *N*-(3,4-dichlorophenyl)acetamide, although the two amides crystallize in different crystal systems.

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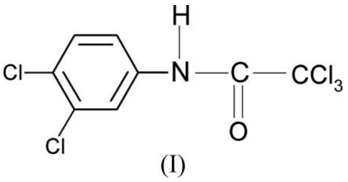
Comment

In the present work, the structure of 2,2,2-trichloro-*N*-(3,4-dichlorophenyl)acetamide (34DCPTCA), (I), has been determined to explore the substituent effects on the structure of *N*-aromatic amides (Gowda *et al.*, 2006, 2007). The substitution of Cl for H atoms in the side-chain methyl group of *N*-(3,4-dichlorophenyl)acetamide (34DCPA) changes the crystal system from triclinic to monoclinic (Jones *et al.*, 1990), but the conformation of the N—H bond continues to be *anti* to the *meta*-Cl substituent (Fig. 1). The substitution in the side chain increases the bond lengths of C4—C5 and C8—N7 from 1.503 (4) to 1.549 (2) Å and 1.409 (3) to 1.424 (2) Å, respectively, but decreases the lengths of C5—O6 and C5—N7 from 1.221 (3) to 1.209 (2) Å and 1.351 (3) to 1.336 (2) Å, respectively. The C5—N7—C8 angle changes from 128.2 (2) to 123.6 (1)° (Table 1). The packing diagram of the title compound, as viewed down the *a* axis, is shown in Fig. 2.



(I)

Experimental

The title compound was prepared according to the literature method (Shilpa & Gowda, 2007). Single crystals of the title compound were obtained by recrystallization from an ethanol solution.

Crystal data

$C_8H_4Cl_5NO$
M_r = 307.37
Monoclinic, $P2_1/c$
a = 5.8610 (2) Å
b = 20.2384 (6) Å
c = 9.9791 (3) Å
β = 104.041 (3)°
V = 1148.33 (6) Å^3
Z = 4
Mo *K*α radiation
μ = 1.23 mm^{-1}
T = 295 (2) K
0.28 × 0.14 × 0.11 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.816, T_{max} = 0.877
15232 measured reflections
2357 independent reflections
2045 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

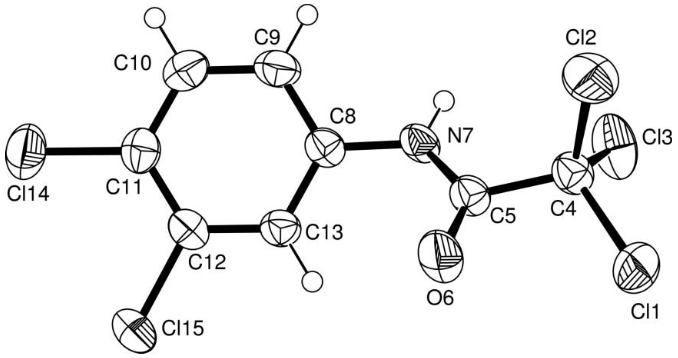


Figure 1
The molecular structure of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.067$
$S = 1.05$
2357 reflections
167 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C4—C5	1.549 (2)	C5—N7	1.336 (2)
C5—O6	1.2092 (18)	C8—N7	1.424 (2)
O6—C5—N7	124.71 (15)	C13—C8—N7	121.37 (14)
O6—C5—C4	119.15 (14)	C9—C8—N7	118.84 (14)
N7—C5—C4	116.05 (13)	C5—N7—C8	123.60 (13)
C13—C8—C9	119.79 (15)		
N7—C8—C9—C10	−178.49 (16)	C13—C8—N7—C5	−40.9 (2)
N7—C8—C13—C12	178.36 (14)	C9—C8—N7—C5	139.49 (17)
C4—C5—N7—C8	−172.72 (14)		

C-bound H atoms were refined using a riding model with C—H distances of 0.93 Å. A restraint of N—H = 0.86 (2) Å was applied for the N-bound H atom. For all H atoms $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N). The title compound exhibits positional disorder of atoms Cl1, Cl2 and Cl3 bonded to atom C4, with the two disorder components rotated relative to each other by about 14°. The C—Cl bond lengths were restrained to 1.76 (1) Å. The refined occupancy factors are 0.56:0.44 (3).

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 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

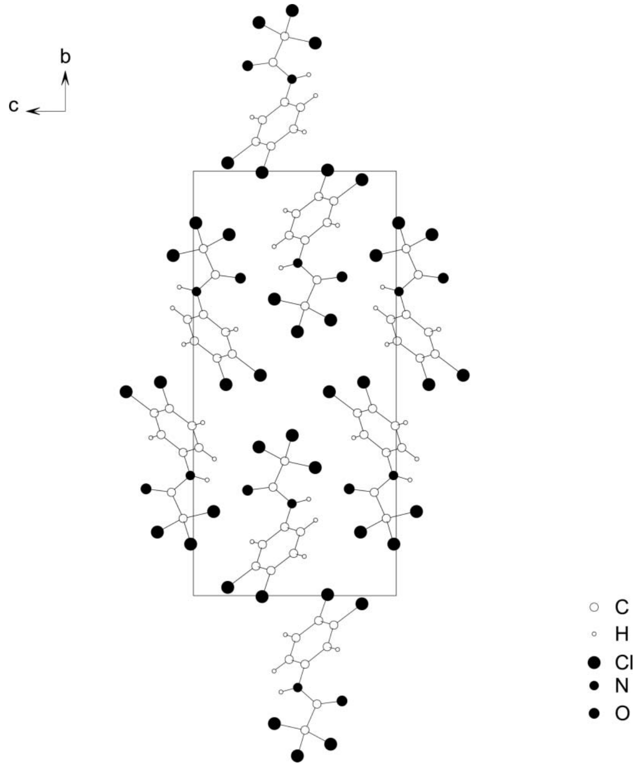


Figure 2
The packing, as viewed down the *a* axis.

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