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2,2,2-Trichloro-*N*-(2,6-dimethylphenyl)acetamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.045
wR factor = 0.131
Data-to-parameter ratio = 12.8

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

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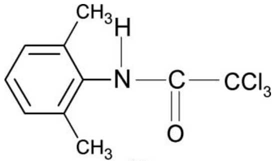
The structure of the title compound, $C_{10}H_{10}Cl_3NO$, is closely related to 2,2,2-trichloro-*N*-phenylacetamide and 2,2,2-trichloro-*N*-(2-methylphenyl)acetamide, with somewhat slightly different bond parameters. The crystal packing is stabilized by an N—H···O hydrogen bond.

Comment

As part of a study to systematize the effect of the substituents on the solid state structures of *N*-aromatic amides (Gowda *et al.*, 2004, 2006; Gowda, Kozisek, Svoboda & Fuess, 2007; Gowda, Paulus *et al.*, 2007; Gowda, Kozisek, Tokarčík & Fuess, 2007), the structure of 2,2,2-trichloro-*N*-(2,6-dimethylphenyl)acetamide, (I), has been determined.



(I)

The structure of (I) (Fig. 1) is closely related to 2,2,2-trichloro-*N*-phenylacetamide (Dou *et al.*, 1994) and 2,2,2-trichloro-*N*-(2-methylphenyl)acetamide (Gowda, Kozisek, Tokarčík & Fuess, 2007), with somewhat slightly different bond parameters. The molecules are linked into chains running along the *c* axis through N—H···O intermolecular hydrogen bonds (Table 1).

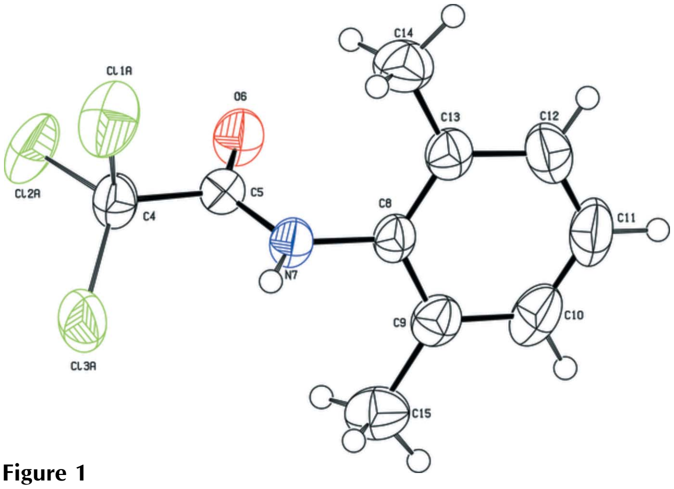


Figure 1
Molecular structure of the title compound showing the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius. Only one disorder component is shown.

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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 IR and NMR spectra (Gowda *et al.*, 2003). Single crystals of the title compound were obtained from a slow evaporation of its ethanol solution.

Crystal data

$C_{10}H_{10}Cl_3NO$
$M_r = 266.54$
Monoclinic, $P2_1/c$
$a = 10.117\ (1)$ Å
$b = 11.898\ (1)$ Å
$c = 10.183\ (1)$ Å
$\beta = 100.89\ (1)^\circ$
$V = 1203.7\ (2)$ Å^3
$Z = 4$
Cu $K\alpha$ radiation
$\mu = 6.68$ mm^{-1}
$T = 299\ (2)$ K
$0.45 \times 0.22 \times 0.10$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.218$, $T_{\max} = 0.514$
4032 measured reflections
2135 independent reflections
1725 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$
3 standard reflections
frequency: 120 min
intensity decay: 2.6%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.131$
$S = 1.08$
2135 reflections
167 parameters
40 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.32$ e Å^{-3}
$\Delta\rho_{\min} = -0.42$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N7—H7N$\cdots$O6$^{\rm i}$	0.856 (10)	2.133 (15)	2.922 (2)	153 (2)
N7—H7N$\cdots$Cl3*A*	0.856 (10)	2.60 (3)	3.025 (6)	112 (2)
N7—H7N$\cdots$Cl3*B*	0.856 (10)	2.68 (3)	2.998 (9)	103 (2)

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

The H atom of the NH group was located in a difference map and refined with a bond length restraint [N—H = 0.86 (1) Å]. The C-bound H atoms were positioned geometrically and treated as riding atoms (C—H = 0.93–0.96 Å). Isotropic displacement parameters for all H atoms were set equal to $1.2U_{\rm eq}$(parent atom).

The Cl atoms are disordered and were refined using a split model. The corresponding site-occupation factors were refined so that their sum was unity [0.60 (2) and 0.40 (2)] and their corresponding bond distances in the disordered groups were restrained to be equal. The U^{ij} components of these atoms were restrained to an approximate isotropic behavior.

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); software used to prepare material for publication: *SHELXL97*.

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