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2,4,5-Trichloroacetanilide

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The title compound, $C_8H_6Cl_3NO$, also known as *N*-(2,4,5-trichlorophenyl)acetamide, is an organic non-linear optical material. It crystallizes in the monoclinic system, in the non-centrosymmetric space group *Pn*.

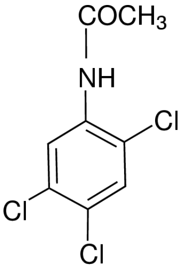
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.023
wR factor = 0.062
Data-to-parameter ratio = 16.4

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

Comment

The title compound, (I), is found to be of interest as an organic non-linear optical material. The crystals show optical second harmonic generation with the fundamental beam (λ = 1064 nm) of an Nd–YAG laser. The single-crystal structure elucidation in a non-centrosymmetric space group further reinforces this observation.



(I)

Fig. 1 shows the title compound. The torsion angle about the C1—N1 bond is 40.3 (3)°, which shows that the amide group deviates markedly from the plane of the phenyl ring (Table 1). The packing of molecules is stabilized by intermolecular N—H···O hydrogen bonds, leading to the formation of molecular chains running along the *a* axis (Fig. 2 and Table 2).

Experimental

The title compound was prepared by the direct reaction of 2,4,5-trichloroaniline and acetic anhydride at room temperature for 10 min. Crystals suitable for single-crystal diffraction study were grown at ambient temperature by slow evaporation of a methanol solution. The title compound crystallizes as colourless needles.

Crystal data

$C_8H_6Cl_3NO$
$M_r = 238.49$
Monoclinic, *Pn*
$a = 3.9015\ (8)$ Å
$b = 12.658\ (3)$ Å
$c = 9.6687\ (19)$ Å
$\beta = 101.186\ (5)^\circ$
$V = 468.42\ (17)$ Å^3
$Z = 2$

$D_x = 1.691$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 825 reflections
$\theta = 3.9$–27.7°
$\mu = 0.93$ mm^{-1}
$T = 293\ (2)$ K
Needle, colourless
0.56 × 0.28 × 0.27 mm

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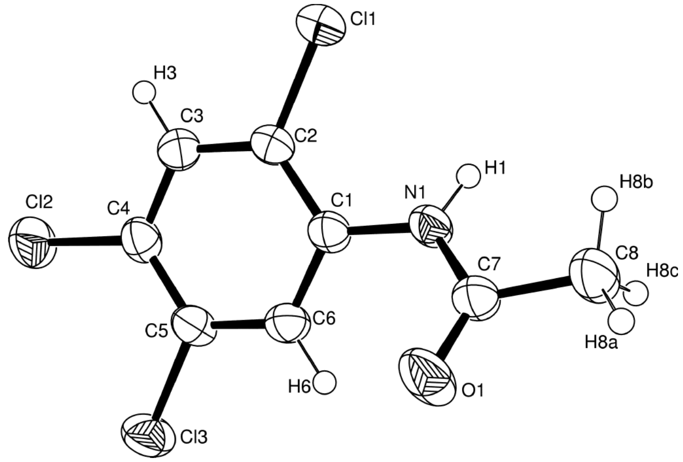

Figure 1
View of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.624$, $T_{\max} = 0.787$
3931 measured reflections
1956 independent reflections
1903 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.014$
$\theta_{\max} = 28.0°$
$h = -5 \rightarrow 5$
$k = -16 \rightarrow 16$
$l = -12 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.062$
$S = 1.05$
1956 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.20$ e Å^{-3}
Absolute structure: (Flack, 1983), 817 Friedel pairs
Flack parameter = 0.04 (4)

Table 1
Selected geometric parameters (Å, °).

Cl1—C2	1.7277 (17)	O1—C7	1.210 (2)
Cl2—C4	1.7256 (16)	N1—C1	1.4067 (19)
Cl3—C5	1.7237 (17)	N1—C7	1.357 (2)
C1—N1—C7	124.18 (14)	Cl2—C4—C5	121.16 (13)
N1—C1—C6	121.22 (14)	Cl3—C5—C4	120.95 (13)
N1—C1—C2	120.58 (14)	Cl3—C5—C6	118.84 (13)
Cl1—C2—C3	118.11 (12)	N1—C7—C8	114.71 (15)
Cl1—C2—C1	120.05 (12)	O1—C7—N1	122.92 (16)
Cl2—C4—C3	118.77 (12)	O1—C7—C8	122.37 (16)
C7—N1—C1—C2	140.98 (18)	C7—N1—C1—C6	−40.3 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1$^{\text{i}}$	0.86	2.19	3.022 (2)	164
C6—H6···O1	0.93	2.46	2.865 (2)	107

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

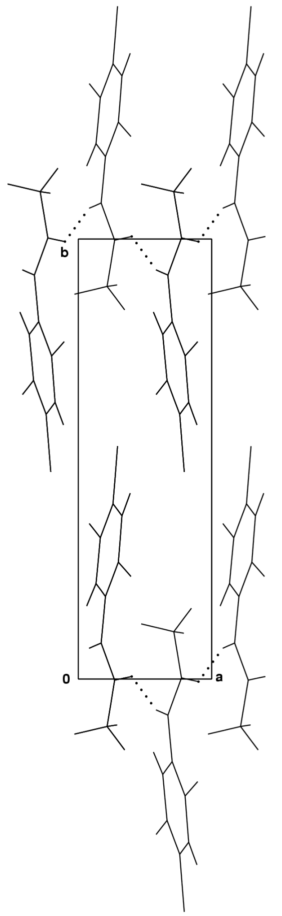

Figure 2
Packing diagram of the title compound, viewed down the *c* axis.

H atoms were refined as riding, with C—H distances of 0.93 or 0.96 Å and an N—H distance of 0.86 Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *PLATON* (Spek, 1990).

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