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2,4,6-Trimethylacetanilide

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Key indicators

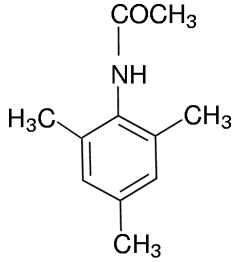
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.116
Data-to-parameter ratio = 17.9

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

The title compound, $C_{11}H_{15}NO$, also known as *N*-(2,4,6-trimethylphenyl)acetamide, is an organic non-linear optical material. It crystallizes in the monoclinic system, in a non-centrosymmetric space group *Pn*.

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 the Nd—YAG laser. The single-crystal structure elucidation in a non-centrosymmetric space group further reinforces this observation.



(I)

Fig. 1 shows the title molecule. The torsion angle about the C1—N1 bond is 71.4 (3)°, showing that the amide group is almost perpendicular to the plane of the phenyl ring (Table 1). The packing shows intermolecular (N—H···O) hydrogen bonds running along [101] (Fig. 2 and Table 2).

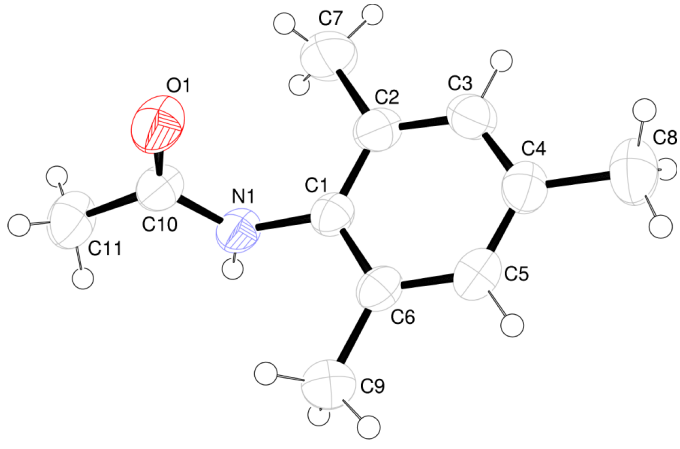


Figure 1
View of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

The title compound, (I), was prepared by the direct reaction of 2,4,6-trimethylaniline and acetic anhydride at room tempertaure for 10 min. Crystals of (I), suitable for single-crystal diffraction study, were grown at ambient temperature by slow evaporation of a methanol solution. The compound crystallizes as colorless prisms.

Crystal data

$C_{11}H_{15}NO$
$M_r = 177.24$
Monoclinic, *Pn*
$a = 8.200$ (4) Å
$b = 8.538$ (4) Å
$c = 8.295$ (4) Å
$\beta = 113.626$ (6)°
$V = 532.1$ (4) Å^3
$Z = 2$
$D_x = 1.106$ Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
Cell parameters from 775 reflections
$\theta = 3.6$–26.2°
$\mu = 0.07$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.52 × 0.44 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
4076 measured reflections
2182 independent reflections
1932 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 28.0°$
$h = -9 \rightarrow 10$
$k = -10 \rightarrow 11$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.116$
$S = 1.13$
2182 reflections
122 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 0.0215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.010$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Absolute structure: Flack (1983), 891 Friedel pairs
Flack parameter = −0.9 (17)

Table 1
Selected geometric parameters (Å, °).

O1—C10	1.233 (2)	N1—C10	1.350 (2)
N1—C1	1.444 (2)		
C1—N1—C10	124.57 (14)	N1—C10—C11	115.19 (15)
N1—C1—C6	118.33 (14)	O1—C10—N1	123.38 (15)
N1—C1—C2	120.71 (15)	O1—C10—C11	121.44 (16)
C10—N1—C1—C2	−71.4 (3)	C10—N1—C1—C6	110.12 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.07	2.899 (2)	162

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

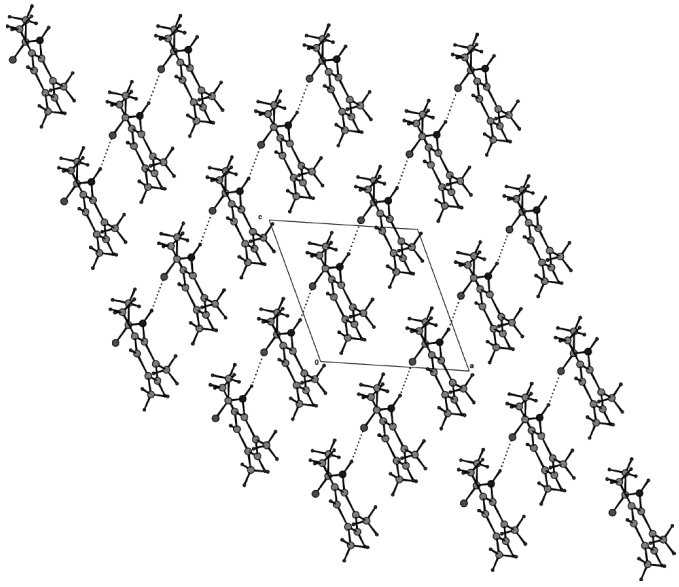


Figure 2
Packing diagram of (I), viewed down the *b* axis.

The absolute configuration could not be determined by the Flack (1983) test. Friedel pairs were merged.

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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References

Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.
Watkin, D. J., Prout, C. K. & Pearce, L. J. (1996). *CAMERON*. Chemical Crystallography Laboratory, University of Oxford, England.