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N-(4-Chlorophenyl)-2,2,2-trimethylacetamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.133
Data-to-parameter ratio = 14.4

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

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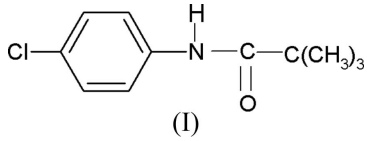
The structure of the title compound, $C_{11}H_{14}ClNO$, is closely related to the ring-unsubstituted 2,2,2-trimethyl-*N*-phenylacetamide and 2,2,2-trimethyl-*N*-(4-methylphenyl)acetamide with slightly different bond parameters. The molecules are linked into chains running along the *b*-axis direction through N—H···O hydrogen bonding.

Comment

In the present work, the structure of *N*-(4-chlorophenyl)-2,2,2-trimethylacetamide (4CPTMA), (I), has been determined as part of a study to systematize the structures of *N*-aromatic amides (Gowda *et al.*, 2004, 2006; Gowda, Kozisek, Svoboda & Fuess, 2007). The structure of 4CPTMA (Fig. 1) is closely related to the ring-unsubstituted 2,2,2-trimethyl-*N*-phenylacetamide (Gowda, Paulus *et al.*, 2007) and 2,2,2-trimethyl-*N*-(4-methylphenyl)acetamide (Gowda, Kozisek, Tokarcik & Fuess, 2007) with similar geometric parameters. In 4CPTMA, the molecules are linked into chains along the *b* axis through N—H···O hydrogen bonds



(I)

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 by slow evaporation of an ethanol solution and used for X-ray diffraction analysis at room temperature.

Crystal data

$C_{11}H_{14}ClNO$
M_r = 211.68
Orthorhombic, *Pbca*
a = 9.6933 (6) Å
b = 10.115 (1) Å
c = 23.542 (1) Å
V = 2308.2 (3) Å^3
Z = 8
Cu *Kα* radiation
μ = 2.67 mm^{-1}
T = 299 (2) K
0.77 × 0.25 × 0.17 mm

Data collection

Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.555, T_{max} = 0.661
2104 measured reflections
2061 independent reflections
1730 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.133$
$S = 1.08$
2061 reflections
143 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7N···O6^{i}	0.84 (2)	2.14 (2)	2.9773 (19)	172 (2)

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, z$.

All C-bound H atoms were positioned geometrically and treated as riding, with C—H = 0.93 (CH aromatic) or 0.96 Å (CH_3) and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The H atom of the NH group was located in a diffrerence map and its position refined [N—H = 0.84 (2) Å and U_{iso}(H) = 1.2U_{eq}(N)].

Data collection: *CAD-4-PC* (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: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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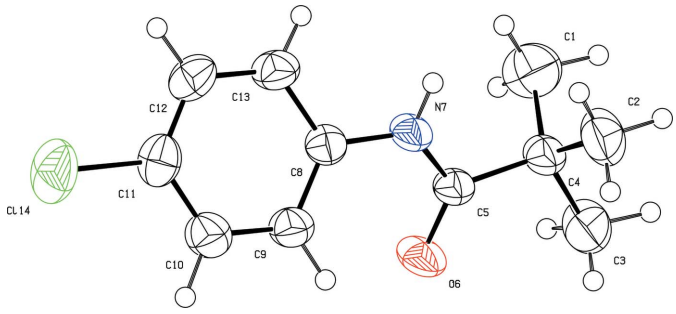

Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radius.

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