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N-(3-Chlorophenyl)-2,2,2-trimethylacetamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.015 Å
R factor = 0.071
wR factor = 0.153
Data-to-parameter ratio = 8.6

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

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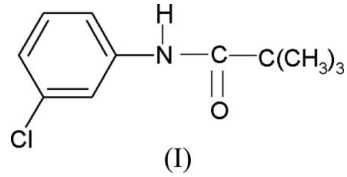
In the structure of the title compound (3CPTMA), $C_{11}H_{14}ClNO$, the conformation of the N—H bond is *anti* to the *meta*-chloro substituent, similar to that observed for the corresponding *meta*-methyl-substituted amide. The bond parameters of the two amides are also similar. The molecules in 3CPTMA are linked into chains, as bent columns, through N—H···O hydrogen bonding.

Comment

The structure of *N*-(3-chlorophenyl)-2,2,2-trimethylacetamide (3CPTMA), (I), has been determined as part of a study on the systematization of the crystal structures of *N*-aromatic amides (Gowda *et al.*, 2004; Gowda, Kozisek & Fuess, 2006; Gowda, Kozisek, Svoboda & Fuess, 2007). In 3CPTMA, the conformation of the N—H bond is *anti* to the *meta*-chloro substituent (Fig. 1), similar to that observed for 2,2,2-trimethyl-*N*-(3-methylphenyl)acetamide (Gowda, Kozisek, Tokarcik & Fuess, 2007). The bond parameters of the two amides and those of the ring-unsubstituted 2,2,2-trimethyl-*N*-phenylacetamide are similar (Gowda, Kozisek, Tokarcik & Fuess, 2007). The molecules in 3CPTMA are linked into chains, as bent columns, through N—H···O hydrogen bonding (Table 1), similar to that observed in other amides (Gowda, Paulus *et al.*, 2007; Gowda, Kozisek, Tokarcik & Fuess, 2007).



(I)

Experimental

The title compound was prepared according to the literature method (Gowda, Shilpa *et al.*, 2006). The purity of the compound was checked by determining its melting point. It was characterized by recording its IR and NMR spectra (Gowda, Shilpa *et al.*, 2006). Single crystals of the title compound were obtained by slow evaporation of an ethanol solution and used for X-ray diffraction studies at room temperature.

Crystal data

$C_{11}H_{14}ClNO$
M_r = 211.68
Orthorhombic, $Pca2_1$
a = 10.778 (1) Å
b = 10.623 (1) Å
c = 10.117 (2) Å
V = 1158.3 (3) Å^3
Z = 4
Cu *Kα* radiation
μ = 2.66 mm^{-1}
T = 299 (2) K
0.68 × 0.05 × 0.03 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.754, T_{max} = 0.855 (expected range = 0.814–0.923)
1745 measured reflections
1095 independent reflections
479 reflections with $I > 2\sigma(I)$
R_{int} = 0.152
3 standard reflections
frequency: 120 min
intensity decay: 5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.153
S = 0.99
1095 reflections
127 parameters
1 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: (Flack, 1983)
Flack parameter: 0.01 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7*N*···O6^{i}	0.86	2.10	2.935 (8)	164

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

All H atoms were positioned geometrically and treated as riding, with C—H = 0.93 (CH aromatic) or 0.96 Å (CH_3) and N—H = 0.86 Å, with U_{iso}(H) = 1.2U_{eq}(C,NH) and 1.5U_{eq}(methyl C).

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* (Farrugia 1997); software used to prepare material for publication: *SHELXL97*.

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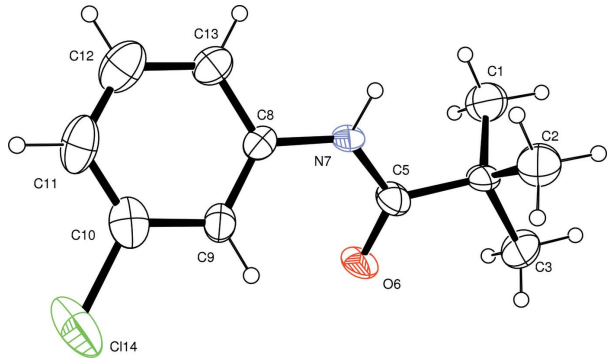

Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radius.

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