Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2,2-Trimethyl-*N*-(4-methylphenyl)acetamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.073
wR factor = 0.202
Data-to-parameter ratio = 15.8

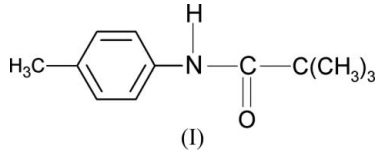
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 21 March 2007
Accepted 28 March 2007

The structure of the title compound, $C_{12}H_{17}NO$, is closely related to the ring-unsubstituted 2,2,2-trimethyl-*N*-phenylacetamide, and *ortho*- and *meta*-ring-substituted amides, with somewhat slightly different bond parameters. N—H···O hydrogen bonding results in the formation of an infinite chain running parallel to the *b* axis.

Comment

As part of a study directed at the systematization of the structures of *N*-aromatic amides (Gowda *et al.*, 2004, 2006, 2007*a*,*b*; Gowda, Kozisek, Svoboda & Fuess, 2007; Gowda, Paulus *et al.*, 2007), the structure of 2,2,2-trimethyl-*N*-(4-methylphenyl)acetamide (4MPTMA), (I), has been determined. The structure of 4MPTMA (Fig. 1) is closely related to the ring-unsubstituted 2,2,2-trimethyl-*N*-phenylacetamide (Gowda, Paulus *et al.*, 2007) and *ortho*/*meta*-ring-substituted amides (Gowda *et al.*, 2007*a*,*b*). The geometric parameters of 4MPTMA are similar to those of the corresponding *ortho*-methyl-substituted (2MPTMA) and *meta*-methyl-substituted (3MPTMA) amides. The dihedral angles between the benzene ring and the amide fragment in the three amides are 55.5 (2) (2MPTMA), 33.0 (1) (3MPTMA) and 32.8 (1)° (4MPTMA).



(I)

As observed in all other related structures, N—H···O hydrogen bonding results in the formation of an infinite chain, running parallel to the *b* axis in this case (Table 1).

Experimental

The title compound was prepared according to the literature method of 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 an ethanol solution and used for X-ray diffraction studies at room temperature.

Crystal data

$C_{12}H_{17}NO$
M_r = 191.27
Orthorhombic, *Pbca*
a = 9.6900 (12) Å
b = 10.1287 (16) Å
c = 23.923 (3) Å
V = 2348.0 (6) Å^3
Z = 8
Mo *Kα* radiation
μ = 0.07 mm^{-1}
T = 299 (2) K
0.32 × 0.19 × 0.09 mm

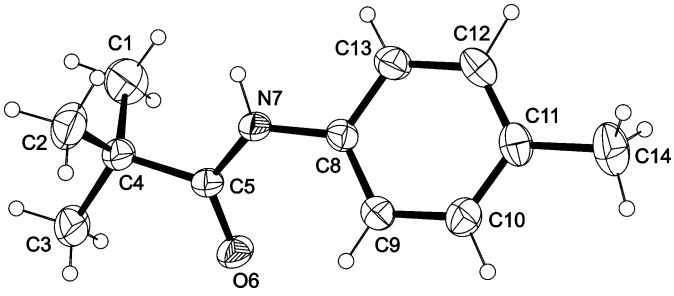


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radius.

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: none
14623 measured reflections
2304 independent reflections
1837 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.202$
$S = 1.23$
2304 reflections
146 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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}	0.87 (2)	2.12 (3)	2.993 (2)	176 (2)

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

All H atoms attached to C 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) = 1.2 U_{eq}(CH) and 1.5 U_{eq}(CH_3). The position of the H atom attached to the N atom was refined freely; U_{iso}(H) = 1.2 U_{eq}(N).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; 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* (Sheldrick, 1997), *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany, for the additional periods of his research fellowship. JK and MT thank the Grant Agency of the Slovak Republic (grant No. 1/2449/05).

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