Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2,2-Trimethyl-*N*-(3-methylphenyl)acetamide

B. Thimme Gowda,[a]* Jozef Kozisek,[b] Miroslav Tokarčík[c] and Hartmut Fuess[d]

[a]Department of Chemistry, Mangalore University, Mangalagangotri-574 199, Mangalore, India, [b]Department of Physical Chemistry, Slovak University of Technology, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, [c]Department of Chemical Physics, Slovak University of Technology, Radlinského 9, 812 37 Bratislava, Slovak Republic, and [d]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287, Darmstadt, Germany

Correspondence e-mail: gowdabt@yahoo.com

Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.102
Data-to-parameter ratio = 9.7

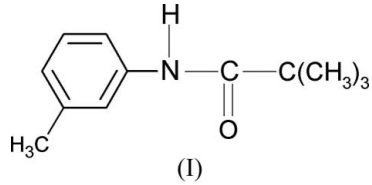
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 March 2007
Accepted 22 March 2007

The conformation of the N—H bond is *anti* to the *meta*-methyl substituent in the structure of the title compound, $C_{12}H_{17}NO$, in contrast to the *ortho*-methyl-substituted amide.

Comment

In the present work, the structure of *N*-(3-methylphenyl)-2,2,2-trimethylacetamide, (I) (3MPTMA), has been determined as part of a study on the systematization of the crystal structures of *N*-aromatic amides (Gowda, Kozisek & Fuess, 2006; Gowda, Shilpa & Jayalakshmi, 2006; Gowda, Kozisek, Svoboda & Fuess, 2007; Gowda, Kozisek, Tokarcik & Fuess, 2007). In 3MPTMA, the conformation of the N—H bond is *anti* to the *meta*-methyl substituent (Fig. 1), in contrast to the *syn* conformation observed for the corresponding *ortho*-methyl-substituted amide (Gowda *et al.*, 2007*b*). The geometric parameters in the two amides are similar, except for the C11—N1—C1 bond angle [124.9 (3)° in 2MPTMA and 127.1 (2)° in 3MPTMA] and the dihedral angles between the benzene ring and the C11—N1—C1—O1—C2 acetamide fragment [55.5 (2)° in 2MPTMA) and 33.0 (1)° in 3MPTMA].



(I)

The molecules of 3MPTMA are linked through N—H···O hydrogen bonds (Table 1), forming chains running along the *c* axis (Fig. 2).

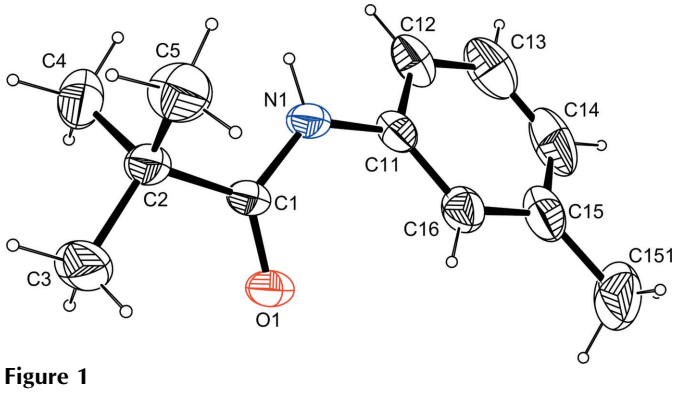


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radius.

Experimental

The title compound was prepared according to a literature method (Gowda, Shilpa & Jayalakshmi, 2006). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Gowda, Shilpa & Jayalakshmi, 2006). Single crystals of the title compound were obtained from an ethanol solution and used for this X-ray diffraction study at room temperature.

Crystal data

$C_{12}H_{17}NO$
M_r = 191.27
Orthorhombic, $Pca2_1$
a = 10.7530 (10) Å
b = 10.8059 (10) Å
c = 10.0883 (11) Å
V = 1172.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 299 (2) K
0.5 × 0.15 × 0.15 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.962, T_{max} = 0.992
7344 measured reflections
1215 independent reflections
765 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.103
S = 0.91
1215 reflections
127 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7···O6^{i}	0.86	2.12	2.954 (3)	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 Å (aromatic) or 0.96 Å (CH_3) and N—H = 0.86 Å, with U_{iso}(H) = 1.2U_{eq}(CH or NH) and U_{iso}(H) = 1.5U_{eq}(CH_3).

In the absence of significant anomalous scattering, Friedel pairs were merged.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); 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).

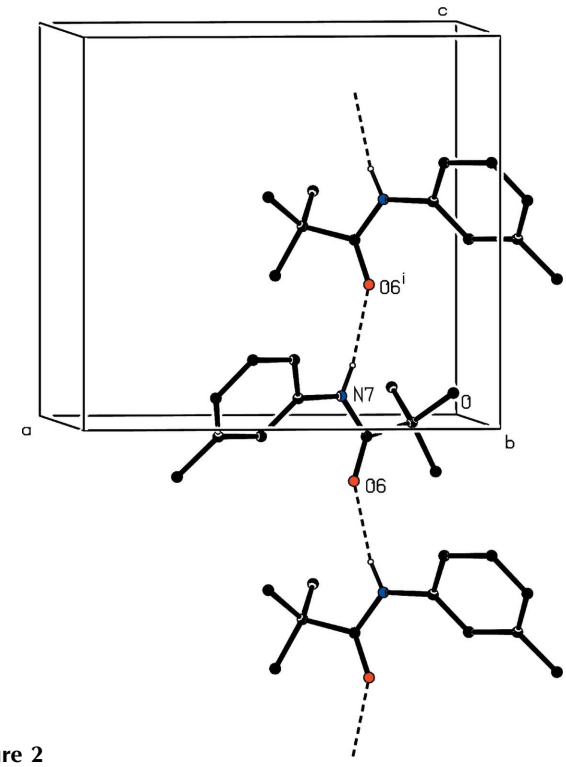


Figure 2
Partial packing view, showing the N—H···O hydrogen bonds linking the molecules into a chain. H bonds are shown as dashed lines. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted. [Symmetry code: (i) $\frac{1}{2}-x, y, \frac{1}{2}+z$]

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

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gowda, B. T., Kozisek, J. & Fuess, H. (2006). *Z. Naturforsch. Teil A*, **61**, 588–594.
Gowda, B. T., Kozisek, J., Svoboda, I. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**, 91–100.
Gowda, B. T., Kozisek, J., Tokarcik, M. T. & Fuess, H. (2007). *Acta Cryst.* E**63**, o1983–o1984.
Gowda, B. T., Shilpa & Jayalakshmi, K. L. (2006). *Z. Naturforsch. Teil A*, **61**, 595–599.
Oxford Diffraction (2003). *CrysAlis CCD*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Oxford Diffraction (2006). *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.