Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(3,5-Dimethylphenyl)acetamide

B. Thimme Gowda,[a]* Jozef Kožíšek,[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

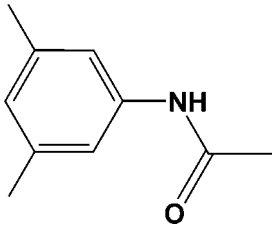
Received 20 April 2007; accepted 20 April 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.066; wR factor = 0.175; data-to-parameter ratio = 15.7.

The structure of the title compound (35DMPA), $C_{10}H_{13}NO$, closely resembles those of *N*-(3,5-dichlorophenyl)acetamide (35DCPA) and other amides. 35DMPA has two molecules in its asymmetric unit, in contrast to the single molecule observed in the asymmetric unit of 35DCPA. In addition, 35DMPA and 35DCPA crystallize in different crystal systems. The molecules in 35DMPA are packed into chains *via* N—H···O hydrogen bonds.

Related literature

For related structures, see: Gowda, Foro & Fuess (2007); Gowda, Kozisek, Svoboda & Fuess (2007); Gowda *et al.* (2007*a*,*b*); Shilpa & Gowda (2007).



Experimental

Crystal data

$C_{10}H_{13}NO$
M_r = 163.21
Monoclinic, $P2_1/c$
a = 8.7925 (12) Å
b = 27.690 (5) Å
c = 7.6525 (15) Å
β = 92.650 (10)°
V = 1861.1 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.31 × 0.26 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
T_{min} = 0.965, T_{max} = 0.991
17320 measured reflections
3638 independent reflections
1750 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.175
S = 0.99
3638 reflections
231 parameters
56 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O1	0.93	2.36	2.865 (4)	114
N1—H1*N*···O2^{i}	0.86	1.96	2.812 (3)	174
C14—H14···O2	0.93	2.33	2.886 (4)	118
N2—H2*N*···O1^{ii}	0.86	1.96	2.810 (3)	167

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); 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*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2166).

References

Clark, R. C. & Reid, J. S. (1995). *Acta Cryst.* A**51**, 887–897.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gowda, B. T., Foro, S. & Fuess, H. (2007). *Acta Cryst.* E**63**, o2341–o2342.
Gowda, B. T., Kozisek, J., Svoboda, I. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**, 91–100.
Gowda, B. T., Kožíšek, J., Tokarčík, M. & Fuess, H. (2007*a*). *Acta Cryst.* E**63**, o1945–o1946.
Gowda, B. T., Kožíšek, J., Tokarčík, M. & Fuess, H. (2007*b*). *Acta Cryst.* E**63**, o2071–o2072.
Oxford Diffraction (2007). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Shilpa & Gowda, B. T. (2007). *Z. Naturforsch. Teil A*, **62**, 84–90.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

 doi:10.1107/S1600536807019812

supplementary materials

Acta Cryst. (2007). E**63**, o2711 [**doi:10.1107/S1600536807019812**]

N-(3,5-Dimethylphenyl)acetamide

B. T. Gowda, J. Kozísek, M. Tokarcík and H. Fuess

Comment

In the present work, the structure of *N*-(3,5-dimethylphenyl)acetamide (35DMPA) has been determined to explore the substituent effects on the structures of N-aromatic amides (Gowda, Foro & Fuess, 2007; Gowda *et al.*, 2007, 2007*a*, 2007*b*). 35DMPA has two molecules in its asymmetric unit (Fig. 1), in contrast to single molecule observed in the asymmetric unit of *N*-(3,5-dichlorophenyl)acetamide (35DCPA). Further, 35DMPA and 35DCPA crystallize in different space group, 35DMPA in monoclinic, P21/c and 35DCPA in orthorhombic, Pna21 (Gowda *et al.*, 2007*b*), respectively. The bond lengths and angles in 35DMPA show normal values. Molecules in 35DMPA form chains by hydrogen bonding, along the base vector [201] (Table 1 and Fig. 2).

Experimental

The title compound was prepared according to the literature method of Shilpa and Gowda (Shilpa & Gowda, 2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared, NMR (Shilpa & Gowda, 2007). Single crystals of the title compound were obtained from a slow evaporation of its ethanolic solution and used for X-ray diffraction studies at room temperature.

Refinement

H atoms were placed geometrically and refined using a riding model with C—H distances of 0.93 Å for the ring hydrogen atoms, 0.96 Å for the methyl groups and 0.86 Å for the NH hydrogen atom.

Figures

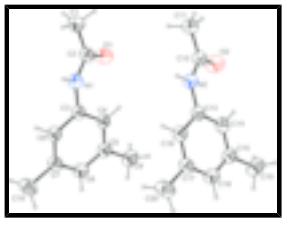


Fig. 1. Molecular structure of (I) showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

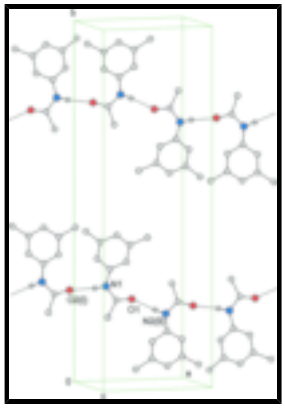


Fig. 2. Part of the crystal structure of (I) showing formation of a chain along the base vector [2 0 1]. H atoms not involved in hydrogen bonding are omitted. Symmetry codes: (i): -1 + *x*,*y*,*z* (ii): *x*,0.5 - *y*,1/2 + *z*

N-(3,5-dimethylphenyl)acetamide

Crystal data

$C_{10}H_{13}NO$	F_{000} = 704
M_r = 163.21	D_x = 1.165 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2654 reflections
a = 8.7925 (12) Å	θ = 3.0–29.5º
b = 27.690 (5) Å	μ = 0.08 mm^{-1}
c = 7.6525 (15) Å	T = 295 (2) K
β = 92.650 (10)º	Block, colourless transparent
V = 1861.1 (6) Å^3	0.31 × 0.26 × 0.08 mm
Z = 8	

Data collection

Xcalibur System, Oxford Diffraction, Ltd. diffractometer	1750 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.076
T = 295(2) K	θ_{max} = 26.0º
φ scans, and ω scans with κ offsets	θ_{min} = 5.1º
Absorption correction: analytical (Clark & Reid, 1995)	h = −10→10
T_{min} = 0.965, T_{max} = 0.991	k = −34→34
17320 measured reflections	l = −9→9
3638 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.066	$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2]$

	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.175$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.99$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
3638 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
231 parameters	Extinction correction: none
56 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1177 (3)	0.19573 (10)	0.7152 (4)	0.0686 (8)
H1A	0.1829	0.178	0.641	0.103*
H1B	0.0196	0.1999	0.6567	0.103*
H1C	0.1066	0.1782	0.8221	0.103*
C2	0.1856 (3)	0.24375 (10)	0.7550 (3)	0.0571 (7)
C3	0.1248 (3)	0.33115 (10)	0.7634 (3)	0.0521 (7)
C4	0.2699 (3)	0.34970 (10)	0.7820 (3)	0.0556 (7)
H4	0.3539	0.3302	0.7642	0.067*
C5	0.2888 (3)	0.39746 (11)	0.8275 (4)	0.0606 (8)
C6	0.1616 (3)	0.42655 (11)	0.8545 (4)	0.0654 (8)
H6	0.1764	0.4586	0.8872	0.079*
C7	0.0158 (3)	0.40896 (11)	0.8341 (4)	0.0628 (8)
C8	0.0000 (3)	0.36131 (11)	0.7880 (3)	0.0584 (7)
H8	−0.0975	0.3485	0.7725	0.07*
C9	0.4470 (3)	0.41717 (12)	0.8490 (4)	0.0808 (10)
H9A	0.5021	0.3998	0.9403	0.121*
H9B	0.4427	0.4508	0.8793	0.121*
H9C	0.4977	0.4135	0.7414	0.121*
C10	−0.1225 (4)	0.44042 (12)	0.8622 (5)	0.0896 (11)
H10A	−0.1969	0.4354	0.7681	0.134*
H10B	−0.0924	0.4738	0.8652	0.134*
H10C	−0.1656	0.432	0.9711	0.134*
O1	0.3102 (2)	0.24743 (7)	0.8168 (3)	0.0835 (7)

N1	0.0982 (2)	0.28246 (8)	0.7227 (3)	0.0581 (6)
H1N	0.0123	0.2766	0.6686	0.07*
C11	0.6329 (3)	0.20839 (10)	0.4921 (4)	0.0673 (8)
H11A	0.6261	0.1979	0.3723	0.101*
H11B	0.5345	0.2061	0.5408	0.101*
H11C	0.7038	0.1883	0.5575	0.101*
C12	0.6859 (3)	0.25926 (10)	0.5005 (3)	0.0570 (7)
C13	0.6067 (3)	0.34252 (10)	0.4195 (3)	0.0524 (7)
C14	0.7468 (3)	0.36566 (11)	0.4156 (3)	0.0609 (8)
H14	0.8353	0.3478	0.4372	0.073*
C15	0.7582 (3)	0.41434 (11)	0.3807 (4)	0.0637 (8)
C16	0.6270 (3)	0.44056 (11)	0.3536 (4)	0.0662 (8)
H16	0.633	0.4735	0.3317	0.079*
C17	0.4852 (3)	0.41861 (11)	0.3583 (4)	0.0616 (8)
C18	0.4771 (3)	0.36980 (11)	0.3900 (3)	0.0582 (7)
H18	0.3823	0.3549	0.3916	0.07*
C19	0.9129 (4)	0.43826 (12)	0.3724 (5)	0.0913 (11)
H19A	0.9569	0.4302	0.2636	0.137*
H19B	0.9783	0.427	0.4678	0.137*
H19C	0.9014	0.4727	0.3805	0.137*
C20	0.3427 (4)	0.44701 (12)	0.3315 (5)	0.0924 (11)
H20A	0.2849	0.4346	0.2318	0.139*
H20B	0.3676	0.4803	0.3116	0.139*
H20C	0.2837	0.4445	0.4335	0.139*
N2	0.5871 (2)	0.29262 (8)	0.4446 (3)	0.0582 (6)
H2N	0.4967	0.2821	0.4198	0.07*
O2	0.8109 (2)	0.27020 (8)	0.5515 (3)	0.0881 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0605 (19)	0.0674 (19)	0.076 (2)	0.0005 (15)	−0.0193 (15)	−0.0054 (15)
C2	0.0450 (18)	0.0666 (19)	0.0580 (18)	0.0047 (15)	−0.0150 (13)	−0.0017 (14)
C3	0.0402 (16)	0.0650 (19)	0.0497 (16)	0.0012 (14)	−0.0127 (12)	0.0051 (13)
C4	0.0363 (15)	0.0679 (19)	0.0617 (17)	0.0008 (13)	−0.0081 (12)	0.0058 (14)
C5	0.0473 (17)	0.071 (2)	0.0624 (18)	−0.0075 (15)	−0.0144 (13)	0.0086 (15)
C6	0.0603 (19)	0.0638 (19)	0.070 (2)	−0.0034 (16)	−0.0170 (15)	0.0000 (15)
C7	0.0484 (18)	0.071 (2)	0.0676 (19)	0.0063 (15)	−0.0132 (14)	0.0010 (15)
C8	0.0393 (16)	0.070 (2)	0.0639 (18)	−0.0022 (14)	−0.0156 (13)	0.0031 (14)
C9	0.0557 (19)	0.086 (2)	0.099 (2)	−0.0193 (17)	−0.0199 (17)	0.0031 (18)
C10	0.066 (2)	0.088 (2)	0.113 (3)	0.0159 (19)	−0.0173 (19)	−0.019 (2)
O1	0.0508 (13)	0.0751 (15)	0.1202 (18)	0.0053 (10)	−0.0443 (12)	0.0007 (12)
N1	0.0388 (13)	0.0666 (15)	0.0665 (15)	−0.0002 (12)	−0.0235 (10)	0.0009 (12)
C11	0.062 (2)	0.069 (2)	0.0695 (18)	0.0019 (16)	−0.0153 (15)	0.0027 (15)
C12	0.0457 (18)	0.072 (2)	0.0519 (17)	0.0032 (15)	−0.0154 (13)	−0.0010 (14)
C13	0.0362 (15)	0.0675 (18)	0.0522 (16)	−0.0022 (14)	−0.0114 (12)	−0.0044 (13)
C14	0.0398 (16)	0.079 (2)	0.0622 (18)	−0.0015 (14)	−0.0139 (13)	0.0002 (14)
C15	0.0537 (18)	0.071 (2)	0.0650 (19)	−0.0126 (16)	−0.0125 (14)	0.0045 (15)

C16	0.062 (2)	0.0641 (19)	0.071 (2)	−0.0038 (16)	−0.0116 (16)	0.0013 (15)
C17	0.0486 (18)	0.070 (2)	0.0643 (19)	0.0029 (15)	−0.0119 (14)	−0.0073 (15)
C18	0.0393 (16)	0.0691 (19)	0.0648 (18)	−0.0050 (14)	−0.0124 (13)	−0.0065 (14)
C19	0.062 (2)	0.098 (3)	0.111 (3)	−0.0287 (19)	−0.0228 (18)	0.022 (2)
C20	0.065 (2)	0.088 (2)	0.121 (3)	0.0169 (19)	−0.0273 (19)	0.000 (2)
N2	0.0366 (13)	0.0624 (15)	0.0735 (15)	−0.0044 (11)	−0.0189 (11)	−0.0011 (12)
O2	0.0526 (14)	0.0954 (16)	0.1113 (17)	−0.0062 (12)	−0.0497 (12)	0.0078 (12)

Geometric parameters (Å, °)

C1—C2	1.483 (4)	C11—C12	1.484 (4)
C1—H1A	0.96	C11—H11A	0.96
C1—H1B	0.96	C11—H11B	0.96
C1—H1C	0.96	C11—H11C	0.96
C2—O1	1.178 (3)	C12—O2	1.189 (3)
C2—N1	1.335 (3)	C12—N2	1.325 (3)
C3—C4	1.377 (3)	C13—C18	1.377 (3)
C3—C8	1.399 (3)	C13—C14	1.390 (3)
C3—N1	1.401 (3)	C13—N2	1.407 (3)
C4—C5	1.375 (4)	C14—C15	1.379 (4)
C4—H4	0.93	C14—H14	0.93
C5—C6	1.401 (4)	C15—C16	1.371 (4)
C5—C9	1.496 (4)	C15—C19	1.517 (4)
C6—C7	1.374 (4)	C16—C17	1.389 (4)
C6—H6	0.93	C16—H16	0.93
C7—C8	1.371 (4)	C17—C18	1.375 (4)
C7—C10	1.519 (4)	C17—C20	1.485 (4)
C8—H8	0.93	C18—H18	0.93
C9—H9A	0.96	C19—H19A	0.96
C9—H9B	0.96	C19—H19B	0.96
C9—H9C	0.96	C19—H19C	0.96
C10—H10A	0.96	C20—H20A	0.96
C10—H10B	0.96	C20—H20B	0.96
C10—H10C	0.96	C20—H20C	0.96
N1—H1N	0.86	N2—H2N	0.86
C2—C1—H1A	109.5	C12—C11—H11A	109.5
C2—C1—H1B	109.5	C12—C11—H11B	109.5
H1A—C1—H1B	109.5	H11A—C11—H11B	109.5
C2—C1—H1C	109.5	C12—C11—H11C	109.5
H1A—C1—H1C	109.5	H11A—C11—H11C	109.5
H1B—C1—H1C	109.5	H11B—C11—H11C	109.5
O1—C2—N1	121.4 (3)	O2—C12—N2	120.7 (3)
O1—C2—C1	121.2 (3)	O2—C12—C11	122.7 (3)
N1—C2—C1	117.3 (2)	N2—C12—C11	116.6 (2)
C4—C3—C8	119.5 (3)	C18—C13—C14	118.1 (3)
C4—C3—N1	121.8 (2)	C18—C13—N2	117.1 (2)
C8—C3—N1	118.7 (2)	C14—C13—N2	124.7 (2)
C5—C4—C3	119.0 (3)	C15—C14—C13	121.8 (3)
C5—C4—H4	120.5	C15—C14—H14	119.1

C3—C4—H4	120.5	C13—C14—H14	119.1
C4—C5—C6	120.1 (3)	C16—C15—C14	118.6 (3)
C4—C5—C9	118.6 (3)	C16—C15—C19	120.8 (3)
C6—C5—C9	121.2 (3)	C14—C15—C19	120.5 (3)
C7—C6—C5	121.8 (3)	C15—C16—C17	121.0 (3)
C7—C6—H6	119.1	C15—C16—H16	119.5
C5—C6—H6	119.1	C17—C16—H16	119.5
C8—C7—C6	116.9 (3)	C18—C17—C16	119.2 (3)
C8—C7—C10	121.1 (3)	C18—C17—C20	119.7 (3)
C6—C7—C10	122.0 (3)	C16—C17—C20	121.1 (3)
C7—C8—C3	122.6 (3)	C17—C18—C13	121.3 (3)
C7—C8—H8	118.7	C17—C18—H18	119.4
C3—C8—H8	118.7	C13—C18—H18	119.4
C5—C9—H9A	109.5	C15—C19—H19A	109.5
C5—C9—H9B	109.5	C15—C19—H19B	109.5
H9A—C9—H9B	109.5	H19A—C19—H19B	109.5
C5—C9—H9C	109.5	C15—C19—H19C	109.5
H9A—C9—H9C	109.5	H19A—C19—H19C	109.5
H9B—C9—H9C	109.5	H19B—C19—H19C	109.5
C7—C10—H10A	109.5	C17—C20—H20A	109.5
C7—C10—H10B	109.5	C17—C20—H20B	109.5
H10A—C10—H10B	109.5	H20A—C20—H20B	109.5
C7—C10—H10C	109.5	C17—C20—H20C	109.5
H10A—C10—H10C	109.5	H20A—C20—H20C	109.5
H10B—C10—H10C	109.5	H20B—C20—H20C	109.5
C2—N1—C3	130.0 (2)	C12—N2—C13	130.3 (2)
C2—N1—H1N	115	C12—N2—H2N	114.9
C3—N1—H1N	115	C13—N2—H2N	114.9
C8—C3—C4—C5	1.1 (4)	C18—C13—C14—C15	−1.1 (4)
N1—C3—C4—C5	−178.0 (2)	N2—C13—C14—C15	176.3 (2)
C3—C4—C5—C6	0.1 (4)	C13—C14—C15—C16	1.7 (4)
C3—C4—C5—C9	179.4 (2)	C13—C14—C15—C19	−178.3 (3)
C4—C5—C6—C7	−1.1 (4)	C14—C15—C16—C17	−1.0 (4)
C9—C5—C6—C7	179.6 (3)	C19—C15—C16—C17	179.0 (3)
C5—C6—C7—C8	0.8 (4)	C15—C16—C17—C18	−0.3 (4)
C5—C6—C7—C10	−179.6 (3)	C15—C16—C17—C20	179.2 (3)
C6—C7—C8—C3	0.5 (4)	C16—C17—C18—C13	0.9 (4)
C10—C7—C8—C3	−179.1 (3)	C20—C17—C18—C13	−178.5 (3)
C4—C3—C8—C7	−1.4 (4)	C14—C13—C18—C17	−0.3 (4)
N1—C3—C8—C7	177.7 (2)	N2—C13—C18—C17	−177.8 (2)
O1—C2—N1—C3	−5.6 (5)	O2—C12—N2—C13	5.9 (4)
C1—C2—N1—C3	172.5 (2)	C11—C12—N2—C13	−172.9 (2)
C4—C3—N1—C2	26.9 (4)	C18—C13—N2—C12	−168.5 (3)
C8—C3—N1—C2	−152.1 (3)	C14—C13—N2—C12	14.1 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O1	0.93	2.36	2.865 (4)	114

N1—H1N···O2^{i}	0.86	1.96	2.812 (3)	174
C14—H14···O2	0.93	2.33	2.886 (4)	118
N2—H2N···O1^{ii}	0.86	1.96	2.810 (3)	167

Symmetry codes: (i) $x-1$, y, z; (ii) x, $-y+1/2$, $z-1/2$.

Fig. 1

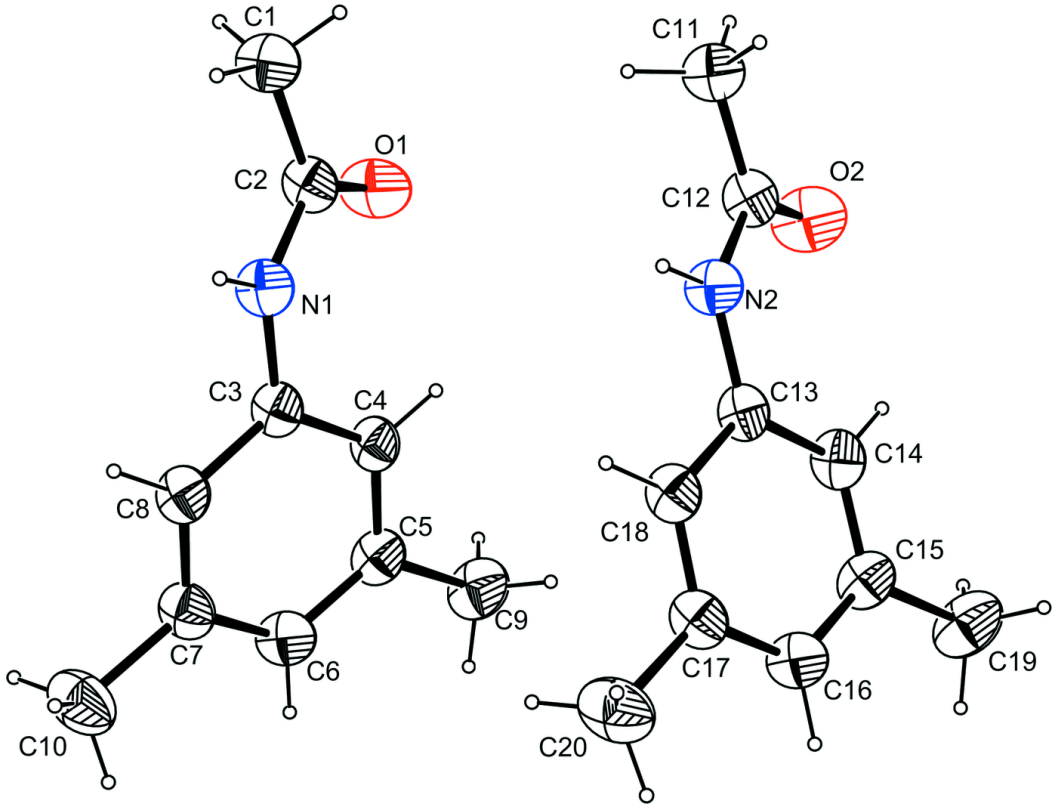

C1
O1
C2
N1
C3
C4
C8
C5
C9
C7
C6
C10
C11
O2
C12
N2
C13
C14
C18
C15
C17
C16
C19
C20

Fig. 2