Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(2,6-Dimethylphenyl)acetamide

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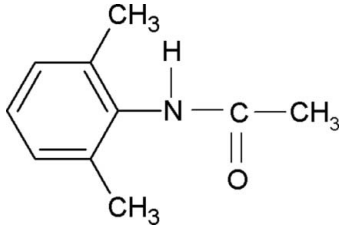
Received 29 May 2007; accepted 1 June 2007

Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.182; data-to-parameter ratio = 15.1.

The structure of the title compound, $C_{10}H_{13}NO$, is closely related to the ring-unsubstituted *N*-phenylacetamide and *N*-(2-methylphenyl)acetamide with slightly different bond parameters. At room temperature it crystallizes in the orthorhombic space group *Pbca*, in contrast with the monoclinic space group $P2_1/n$ observed for the low-temperature structure of the compound. The molecules are linked into chains running along the *a*-axis direction through N—H···O hydrogen bonding.

Related literature

For related literature, see: Brown (1966); Gowda *et al.* (2004, 2007); Gowda, Foro & Fuess (2007*a*,*b*); Gowda *et al.*, 2007; Gowda, Kožíšek, Tokarčík & Fuess (2007*a*,*b*); Hanson *et al.* (2004); Nagarajan *et al.* (1986).



Experimental

Crystal data

$C_{10}H_{13}NO$
M_r = 163.21
Orthorhombic, *Pbca*
a = 9.145 (1) Å
b = 13.215 (1) Å
c = 15.993 (1) Å
V = 1932.8 (3) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 299 (2) K
0.50 × 0.13 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.742, T_{max} = 0.944
1917 measured reflections
1710 independent reflections
1055 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
3 standard reflections
frequency: 120 min
intensity decay: 2.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.182
S = 1.03
1710 reflections
113 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4N···O3^{i}	0.854 (10)	1.986 (10)	2.838 (2)	175 (2)

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

Data collection: *CAD-4-PC* (Enraf–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: *PLATON* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

BTG gratefully thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2089).

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supplementary materials

Acta Cryst. (2007). E**63**, o3154 [**doi:10.1107/S1600536807027031**]

N-(2,6-Dimethylphenyl)acetamide

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Comment

Amides are of fundamental chemical interest as conjugation between the nitrogen lone pair electrons and the carbonyl pi-bond results in distinct physical and chemical properties. Further the amide moiety is an important constituent of many biologically significant compounds. Thus the structural studies of amides are of interest(Brown, 1966; Nagarajan *et al.*, 1986; Hanson *et al.*, 2004; Gowda, Foro & Fuess, 2007*a*,*b*; Gowda *et al.*, 2007; Gowda, Kozisek, Tokarcik & Fuess, 20 07*a*,b). In the present work, the structure of *N*-(2,6-dimethylphenyl)-acetamide (26DMPA) has been determined at 299 (2) K, as part of our study of the effect of ring and side chain substitutions on the solid state geometry of chemically and biologically significant compounds such as acetanilides (Gowda, Foro & Fuess, 2007*a*,*b*; Gowda *et al.*, 2007; Gowda, Kozisek, Tokarcik & Fuess, 2007*a*,b). The present high temperature structure (299 (2) K) crystallizes in orthorhombic Pbca space group, in contrast to the monoclinic $P2_1/n$ space group (Z = 4, a = 7.6836 (6) Å, b = 16.0769 (11) Å, c = 8.1209 (4) Å, beta = 111.881 (4)°) low temperature (173 K) structure of the compound (Hanson *et al.*, 2004). The molecules in the title compound are linked into chains as layers running along the *a* axis direction through N—H···O hydrogen bonding (Table 1, Fig.2).

Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2004). The purity of the compound was checked by determining its melting point. The compound was further characterized by recording its infrared and NMR spectra (Gowda *et al.*, 2004). Single crystals of the title compound were obtained from a slow evaporation of an ethanolic solution and used for X-ray diffraction studies at room temperature.

Refinement

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

Figures

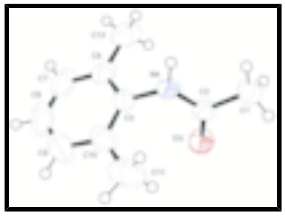

Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

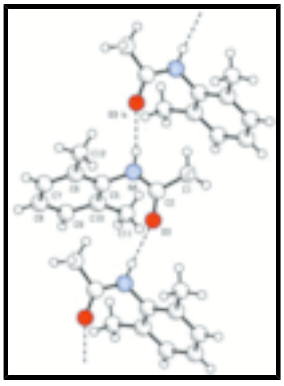

Fig. 2. Typical Hydrogen bond bridges observed in the title compound

N-(2,6-Dimethylphenyl)acetamide

Crystal data

$C_{10}H_{13}NO$	F_{000} = 704
M_r = 163.21	D_x = 1.122 Mg m^{-3}
Orthorhombic, *Pbca*	Cu *Kα* radiation λ = 1.54180 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 25 reflections
a = 9.1450 (10) Å	θ = 6.7–22.2º
b = 13.2150 (10) Å	μ = 0.57 mm^{-1}
c = 15.9930 (10) Å	*T* = 299 (2) K
V = 1932.8 (3) Å^3	Prism, colourless
Z = 8	0.50 × 0.13 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.027
Radiation source: fine-focus sealed tube	θ_{max} = 66.9º
Monochromator: graphite	θ_{min} = 5.5º
T = 299(2) K	*h* = 0→10
ω/2θ scans	*k* = −15→2
Absorption correction: Psi-scan (North *et al.*, 1968)	*l* = 0→19
T_{min} = 0.742, T_{max} = 0.944	3 standard reflections
1917 measured reflections	every 120 min
1710 independent reflections	intensity decay: 2.5%
1055 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.056	H atoms treated by a mixture of

	independent and constrained refinement
$wR(F^2) = 0.182$	$w = 1/[\sigma^2(F_o^2) + (0.104P)^2 + 0.094P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.004$
1710 reflections	$\Delta\rho_{max} = 0.20$ e Å^{-3}
113 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
1 restraint	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0014 (5)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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	0.2449 (3)	0.9101 (3)	0.13523 (16)	0.0651 (8)
H1A	0.2285	0.9810	0.1265	0.078*
H1B	0.2245	0.8739	0.0845	0.078*
H1C	0.3450	0.8992	0.1510	0.078*
C2	0.1469 (2)	0.87292 (19)	0.20292 (14)	0.0464 (6)
C5	0.1374 (2)	0.8040 (2)	0.34433 (15)	0.0479 (6)
C6	0.1394 (3)	0.8645 (2)	0.41568 (16)	0.0599 (8)
C7	0.0703 (3)	0.8280 (3)	0.48692 (18)	0.0833 (11)
H7	0.0714	0.8665	0.5356	0.100*
C8	0.0014 (4)	0.7376 (4)	0.4867 (3)	0.1018 (15)
H8	−0.0452	0.7150	0.5349	0.122*
C9	−0.0005 (4)	0.6788 (3)	0.4160 (3)	0.0957 (13)
H9	−0.0481	0.6166	0.4170	0.115*
C10	0.0680 (3)	0.7109 (2)	0.3426 (2)	0.0686 (9)
C11	0.0652 (5)	0.6467 (2)	0.2660 (3)	0.0986 (13)
H11A	0.0245	0.5817	0.2794	0.118*
H11B	0.1630	0.6383	0.2454	0.118*
H11C	0.0063	0.6788	0.2240	0.118*
C12	0.2110 (4)	0.9663 (3)	0.41539 (19)	0.0813 (10)
H12A	0.1599	1.0103	0.3775	0.098*
H12B	0.3108	0.9596	0.3978	0.098*
H12C	0.2080	0.9945	0.4707	0.098*

N4	0.21296 (19)	0.83891 (16)	0.27191 (12)	0.0473 (5)
H4N	0.3045 (12)	0.8486 (18)	0.2789 (15)	0.057*
O3	0.01362 (17)	0.87350 (17)	0.19453 (10)	0.0639 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0379 (12)	0.097 (2)	0.0600 (15)	−0.0013 (14)	0.0082 (11)	0.0107 (16)
C2	0.0257 (11)	0.0619 (15)	0.0515 (14)	0.0041 (11)	0.0023 (9)	−0.0031 (12)
C5	0.0282 (10)	0.0649 (16)	0.0504 (13)	0.0041 (11)	−0.0019 (10)	0.0103 (13)
C6	0.0312 (12)	0.096 (2)	0.0526 (15)	0.0082 (14)	−0.0042 (10)	0.0043 (15)
C7	0.0518 (17)	0.147 (4)	0.0515 (16)	0.007 (2)	0.0011 (13)	0.012 (2)
C8	0.064 (2)	0.163 (4)	0.079 (2)	0.000 (3)	0.0123 (19)	0.055 (3)
C9	0.069 (2)	0.103 (3)	0.114 (3)	−0.018 (2)	−0.002 (2)	0.054 (3)
C10	0.0502 (16)	0.0663 (18)	0.089 (2)	−0.0030 (15)	−0.0024 (15)	0.0177 (18)
C11	0.101 (3)	0.0607 (18)	0.134 (3)	−0.012 (2)	−0.009 (2)	−0.008 (2)
C12	0.068 (2)	0.101 (3)	0.0740 (19)	−0.003 (2)	−0.0031 (16)	−0.0269 (19)
N4	0.0229 (8)	0.0694 (13)	0.0497 (11)	−0.0020 (10)	−0.0016 (8)	0.0018 (10)
O3	0.0241 (9)	0.1064 (17)	0.0612 (11)	0.0028 (9)	−0.0014 (7)	0.0110 (11)

Geometric parameters (Å, °)

C1—C2	1.489 (3)	C8—C9	1.372 (6)
C1—H1A	0.9600	C8—H8	0.9300
C1—H1B	0.9600	C9—C10	1.397 (5)
C1—H1C	0.9600	C9—H9	0.9300
C2—O3	1.226 (3)	C10—C11	1.489 (5)
C2—N4	1.336 (3)	C11—H11A	0.9600
C5—C10	1.385 (4)	C11—H11B	0.9600
C5—C6	1.394 (4)	C11—H11C	0.9600
C5—N4	1.425 (3)	C12—H12A	0.9600
C6—C7	1.390 (4)	C12—H12B	0.9600
C6—C12	1.496 (4)	C12—H12C	0.9600
C7—C8	1.350 (6)	N4—H4N	0.854 (10)
C7—H7	0.9300		
C2—C1—H1A	109.5	C8—C9—C10	121.1 (4)
C2—C1—H1B	109.5	C8—C9—H9	119.5
H1A—C1—H1B	109.5	C10—C9—H9	119.5
C2—C1—H1C	109.5	C5—C10—C9	117.2 (3)
H1A—C1—H1C	109.5	C5—C10—C11	122.0 (3)
H1B—C1—H1C	109.5	C9—C10—C11	120.7 (3)
O3—C2—N4	122.8 (2)	C10—C11—H11A	109.5
O3—C2—C1	121.1 (2)	C10—C11—H11B	109.5
N4—C2—C1	116.1 (2)	H11A—C11—H11B	109.5
C10—C5—C6	122.2 (2)	C10—C11—H11C	109.5
C10—C5—N4	119.6 (3)	H11A—C11—H11C	109.5
C6—C5—N4	118.2 (2)	H11B—C11—H11C	109.5
C7—C6—C5	117.8 (3)	C6—C12—H12A	109.5

C7—C6—C12	120.9 (3)	C6—C12—H12B	109.5
C5—C6—C12	121.3 (2)	H12A—C12—H12B	109.5
C8—C7—C6	121.2 (4)	C6—C12—H12C	109.5
C8—C7—H7	119.4	H12A—C12—H12C	109.5
C6—C7—H7	119.4	H12B—C12—H12C	109.5
C7—C8—C9	120.5 (3)	C2—N4—C5	124.13 (18)
C7—C8—H8	119.7	C2—N4—H4N	120.0 (17)
C9—C8—H8	119.7	C5—N4—H4N	114.7 (17)
C10—C5—C6—C7	0.8 (4)	N4—C5—C10—C9	178.0 (2)
N4—C5—C6—C7	−177.6 (2)	C6—C5—C10—C11	179.6 (3)
C10—C5—C6—C12	−178.0 (3)	N4—C5—C10—C11	−2.0 (4)
N4—C5—C6—C12	3.6 (3)	C8—C9—C10—C5	0.1 (5)
C5—C6—C7—C8	−1.0 (4)	C8—C9—C10—C11	−179.9 (3)
C12—C6—C7—C8	177.8 (3)	O3—C2—N4—C5	−2.9 (4)
C6—C7—C8—C9	0.7 (5)	C1—C2—N4—C5	177.6 (3)
C7—C8—C9—C10	−0.2 (6)	C10—C5—N4—C2	73.7 (3)
C6—C5—C10—C9	−0.4 (4)	C6—C5—N4—C2	−107.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4N···O3^{i}	0.854 (10)	1.986 (10)	2.838 (2)	175 (2)

Symmetry codes: (i) *x*+1/2, *y*, −*z*+1/2.

Fig. 1

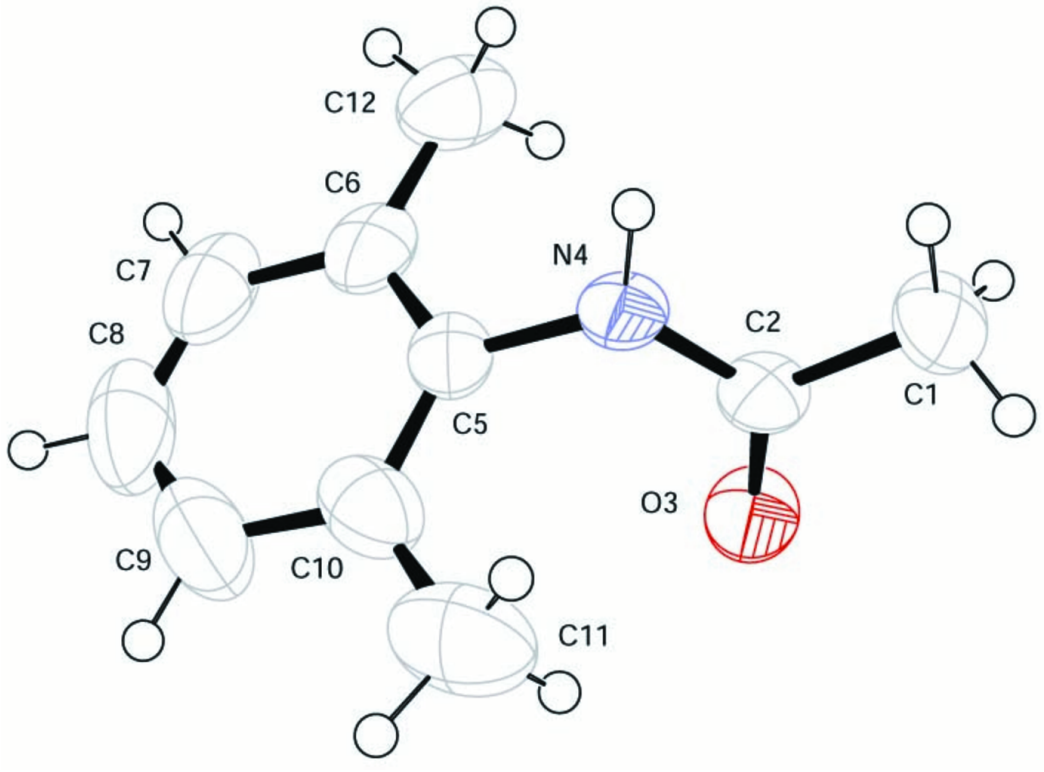

Fig. 2