Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

N-(1-Naphthyl)formamide

Bernard Omondi,* Demetrius C. Levendis and Nerona Naidoo

Molecular Science Institute, School of Chemistry, University of the Witwatersrand, PO Wits, 2050 Johannesburg, South Africa

Correspondence e-mail:
bernard@chem.wits.ac.za

Received 20 December 2006
Accepted 9 January 2007

In the title molecule, $C_{11}H_9NO$, all bond lengths and angles are normal. The crystal structure is stabilized by intermolecular N—H···O and C—H···O hydrogen bonds and π–π stacking interactions.

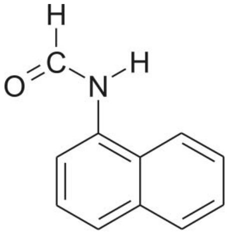
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.030
wR factor = 0.080
Data-to-parameter ratio = 10.1

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

Comment

N-Phenylformamides display a variety of packing patterns (Taylor & Kennard, 1982, 1983; Taylor *et al.*, 1983; 1984*a*,*b*; Leiserowitz & Tuval, 1978). In continuation of our systematic study of disubstituted *N*-phenylformamides in the crystalline state (Omondi *et al.*, 2005; Omondi, 2006), we present here the crystal structure of the title compound, (I).



(I)

In compound (I) (Fig. 1), all bond lengths and angles are normal (Allen *et al.*, 1987). The C2—C1—N1—C11 torsion angle is 53.0 (2)°. The orientation of the formamide unit in (I) is similar to that observed in 2,6-disubstituted phenylformamides (Omondi *et al.*, 2005), but different from that found in *N*-2-naphthylacetamide (Haisa *et al.*, 1980). In the latter structure, the naphthyl and acetamide fragments are almost coplanar and form sheets of hydrogen-bonded molecules.

In the crystal structure of (I) (Fig. 2), N—H···O hydrogen bonds (Table 1) link the molecules into chains running along the short *a* axis. The molecules in the chains are related by translation; the naphthyl ring systems are stacked parallel to each other, with a relatively short $Cg1\cdots Cg2^{iii}$ distance of 3.759 (1) Å, corresponding to π–π intermolecular interactions [*Cg*1 and *Cg*2 are the centroids of the C1–C5/C10 and C5–C10 rings, respectively; symmetry code: (iii) $-1 + x, y, z$]. Weak intermolecular C—H···O hydrogen bonds (Table 1) contribute to the stability of the crystal packing.

Using the *OPIX* suite of programs (Gavezzotti, 2003), the lattice energy of (I) was calculated to be −118.36 kJ mol^{-1}. These calculations allowed us to estimate the quantitative contributions to this energy of the N—H···O, π–π and C—H···O intermolecular interactions as −49.97, −14.40 and −13.96 kJ mol^{-1}, respectively.

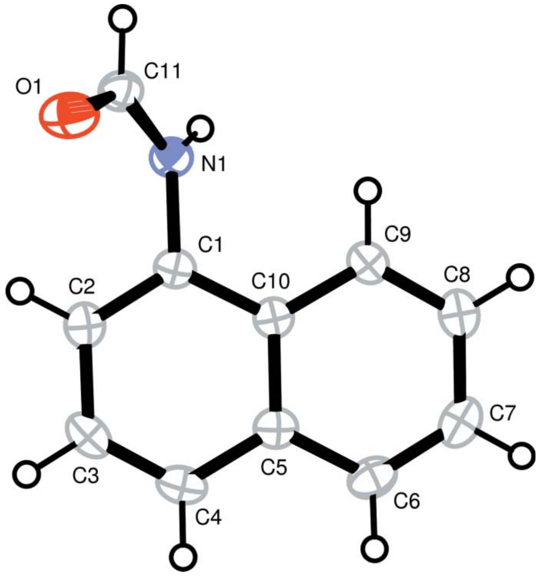


Figure 1
The molecular structure of (I), showing the atomic numbering scheme and 50% probability displacement ellipsoids.

Experimental

N-Naphthalenylformamide was synthesized following a known procedure (Ugi *et al.*, 1965). Commercially available 1-naphthylamine (Aldrich, purity > 95%) was heated in a tenfold excess of formic acid for a period of 15 h at 363 K. The excess formic acid was then removed under vacuum to give a purple solid, which was treated with dilute hydrochloric acid (0.1 *M* HCl, 10 ml) and ethyl acetate (60 ml). The organic layer was separated from the aqueous layer, dried over magnesium sulfate and filtered. Purple needle-shaped crystals of *N*-naphthylenyl-1-formamide were grown from the filtrate.

Crystal data

$C_{11}H_9NO$
$M_r = 171.19$
Orthorhombic, $P2_12_12_1$
$a = 4.4639\ (2)$ Å
$b = 11.8463\ (3)$ Å
$c = 15.8514\ (4)$ Å
$V = 838.23\ (5)$ Å^3
$Z = 4$
$D_x = 1.357$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 173\ (2)$ K
Needle, purple
0.6 × 0.09 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.930$, $T_{max} = 0.992$
14873 measured reflections
1236 independent reflections
1097 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 28.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.080$
$S = 1.06$
1236 reflections
122 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.1116P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

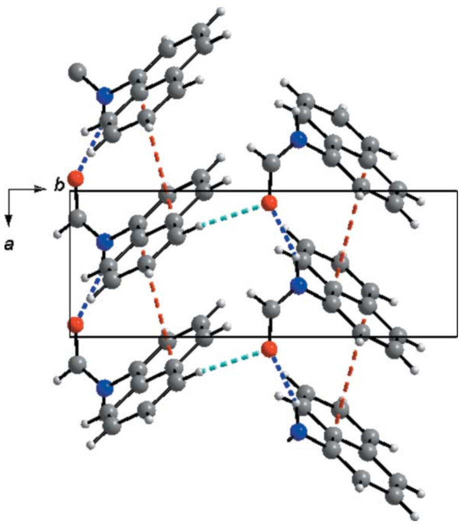


Figure 2
A portion of the crystal packing of (I), viewed down the *c* axis. Dashed lines denote hydrogen bonds and π–π stacking interactions.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.85 (3)	2.00 (2)	2.7971 (19)	155.3 (18)
C6—H6···O1^{ii}	0.95	2.50	3.436 (2)	170

Symmetry codes: (i) $x + 1, y, z$; (ii) $-x, y - \frac{1}{2}, -z + \frac{3}{2}$.

C-bound H atoms were positioned geometrically, with C—H = 0.95 Å, and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. The N-bound atom H1 was located in a difference map and refined isotropically. In the absence of any significant anomalous scatterers in the molecule, the 826 Friedel pairs were merged before the final refinement.

Lattice energy calculations were performed using the *ZIPOPEC* module of the *OPIX* program suite (Gavezzotti, 2003).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003), *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the National Research Foundation (NRF; grant No. GUN 2067413), the IUCr for a PhD grant for BO, and the University of the Witwatersrand.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Brandenburg, K. (2006). *DIAMOND*. Release 3.1d. Crystal Impact GbR, Bonn, Germany.
Bruker (1997). *SMART* (Version 5.6) and *SAINT* (Version 5.06a). Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gavezzotti, A. (2003). *OPIX*. University of Milan, Italy.

Acta Cryst. (2007). E**63**, o714–o716 Omondi *et al.* • $C_{11}H_9NO$ **o715**

Haisa, M., Kashino, S., Ueno, T., Shinozaki, N. & Matsuzaki, Y. (1980). *Acta Cryst.* B**36**, 2306–2311.

Leiserowitz, L. & Tuval, M. (1978). *Acta Cryst.* B**34**, 1230–1247.

Omondi, B. (2006). PhD thesis. Submitted to The University of the Witwatersrand, Johannesburg, South Africa.

Omondi, B., Fernandes, M. A., Layh, M., Levendis, D. C., Mkwizu, T. & Look, J. (2005). *CrystEngComm*, **7**, 690–700.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Taylor, R. & Kennard, O. (1982). *J. Am. Chem. Soc.* **104**, 5063–5070.

Taylor, R. & Kennard, O. (1983). *Acta Cryst.* B**39**, 133–138.

Taylor, R., Kennard, O. & Versichel, W. (1983). *J. Am. Chem. Soc.* **105**, 5761–5766.

Taylor, R., Kennard, O. & Versichel, W. (1984*a*). *J. Am. Chem. Soc.* **106**, 244–248.

Taylor, R., Kennard, O. & Versichel, W. (1984*b*). *Acta Cryst.* B**40**, 280–288.

Ugi, I., Fetzer, U., Eholzer, U., Knupfer, H. & Offermann, K. (1965). *Angew. Chem. Int. Ed. Engl.* **4**, 472–484.

o716 Omondi *et al.* • $C_{11}H_9NO$ *Acta Cryst.* (2007). E**63**, o714–o716