Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(2-Nitro-4-propoxyphenyl)acetamide

H. S. Yathirajan,[a] S. Bindya,[a] M. A. Ashok,[a] B. Narayana[b] and Michael Bolte[c]*

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [b]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [c]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany

Correspondence e-mail: bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.105
Data-to-parameter ratio = 15.2

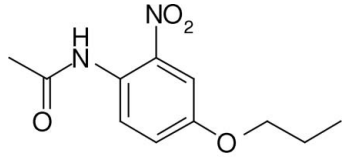
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 22 March 2007
Accepted 29 March 2007

The title compound, $C_{11}H_{14}N_2O_4$, has an almost planar molecule, whose conformation is stabilized by an intramolecular N—H···O hydrogen bond.

Comment

Acetamide derivatives are used as inhibitors of peroxides and stabilizers for cellulose ester varnishes and as anticonvulsants (Soyer *et al.*, 2004), antibacterials (Gregoriou *et al.*, 1977) and radiation-protective agents (Nander & Oberdorfer, 2002). The crystal structure of *N*-[4-(4-nitrobenzylideneamino)phenyl]-acetamide has been reported (Wu *et al.*, 2006). The structures of the potential non-linear optical (NLO) materials *N*-[2-(isopropylamino)-5-nitrophenyl]acetamide and *N*-[2-(butylamino)-5-nitrophenyl]acetamide have been investigated by X-ray crystallographic analysis (Clark *et al.*, 2000). The crystal structures of an important medicinal intermediate, *N*-(4-fluorophenyl)acetamide (Li *et al.*, 2006), and a potential antiamnesic agent, *N*-[4-(morpholinocarbonylmethoxy)phenyl]acetamide monohydrate (Sundar *et al.*, 2006), have also been reported. In view of the importance of acetamide derivatives in general and the title compound, (I), as a pharmaceutical intermediate in particular, the present paper reports the crystal structure of the title compound.



(I)

The molecular structure of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.28, November 2006; updated January 2007; Allen, 2002; *Mogul* Version 1.1; Bruno *et al.*, 2004). Molecules of the title compound are almost planar (r.m.s. deviation for all non-H atoms 0.241 Å). All substituents are slightly twisted out of the plane of the aromatic ring (Table 1). The molecular conformation is stabilized by an intramolecular N—H···O hydrogen bond (Table 2).

Experimental

The title compound was obtained as a gift sample from Arvee Chem Pharma, Mysore. X-ray quality crystals were obtained from methanol by slow evaporation (m.p. 365 K).

Crystal data

$C_{11}H_{14}N_2O_4$
M_r = 238.24
Monoclinic, $P2_1/c$
a = 16.9055 (15) Å
b = 4.0057 (2) Å
c = 18.0989 (16) Å
β = 111.490 (7)°
V = 1140.42 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 173 (2) K
0.31 × 0.26 × 0.08 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: none
15998 measured reflections
2437 independent reflections
2090 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 1.06
2437 reflections
160 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected torsion angles (°).

C2—C1—N1—C11	−156.72 (13)	C5—C4—O4—C41	−177.70 (11)
C1—N1—C11—C12	177.17 (13)	C4—O4—C41—C42	167.94 (11)
C3—C2—N2—O22	−10.23 (17)	O4—C41—C42—C43	177.53 (11)
C1—C2—N2—O21	−11.35 (19)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O21	0.91 (2)	1.96 (2)	2.6554 (15)	132.4 (17)

Carbon-bound H atoms were found in a difference map, but they were refined using a riding model, with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate but not to tip. The N-bound H atom was freely refined.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

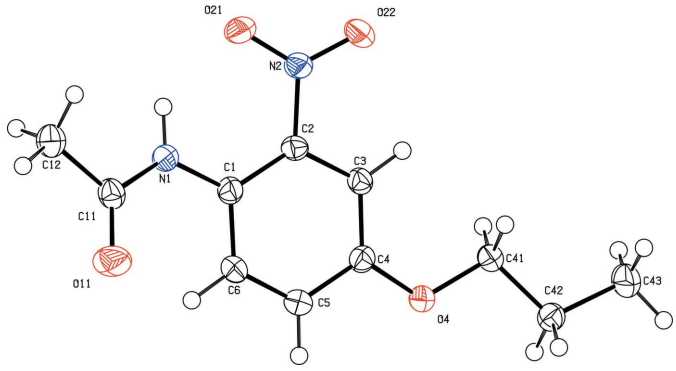


Figure 1
The molecular structure of the title compound, showing the atom numbering and displacement ellipsoids drawn at the 50% probability level.

One of the authors (SB) thanks the University of Mysore for permission to carry out the research work.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruno, I. J., Cole, J. C., Kessler, M., Luo, J., Motherwell, W. D. S., Purkis, L. H., Smith, B. R., Taylor, R., Cooper, R. I., Harris, S. E. & Orpen, A. G. (2004). *J. Chem. Inf. Comput. Sci.* **44**, 2133–2144.
Clark, R. D., Romero, A., Borbulevych, O. Ya., Antipin, M. Yu., Nesterov, V. N. & Timofeeva, T. V. (2000). *Acta Cryst.* C**56**, 336–338.
Gregoriou, M., Brown, P. R. & Tata, R. (1977). *J. Bacteriol.* **132**, 377–384.
Li, D. C., Zhou, W. Y. & Li, C. B. (2006). *Acta Cryst.* E**62**, o66–o67.
Nander, M. W. & Oberdorfer, F. (2002). *Appl. Radiat. Isot.* **57**, 681–685.
Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Soyer, Z., Kilic, F. S., Erol, K. & Pabaccuoglu, V. (2004). *Arch. Pharm.* **337**, 105–111.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Sundar, T. V., Parthasarathi, V., Lang, H., Malik, R. & Piplani, P. (2006). *Acta Cryst.* E**62**, o1874–o1876.
Wu, Y., Zhao, B. & Li, B. (2006). *Acta Cryst.* E**62**, o5677–o5678.