Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-Benzyl-2-(4-nitrophenoxy)acetamide

Yu-Liang Zhang[a]* and Xiao-Hui Li[b]

[a]Department of Chemistry, East China University of Science and Technology, Shanghai 200237, People's Republic of China, and [b]Department of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China

Correspondence e-mail: yuliang_zhang@sohu.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.130
Data-to-parameter ratio = 14.7

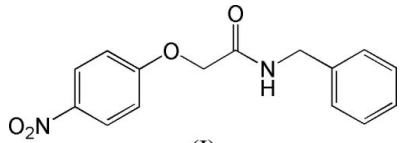
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 5 January 2007
Accepted 11 January 2007

There are two independent molecules in the asymmetric unit of the title compound, $C_{15}H_{14}N_2O_4$, which differ from each other in some torsion angles. In the crystal structure, molecules are linked throgh intermolecular N—H···O hydrogen bonds, forming chains running along the *b* axis.

Comment

Much attention has been focused on amide-type compounds and their metal ion complexes for their properties and potential applications including molecular recognition, ion electrodes, photochemistry and topological structures in ion extraction, biochemistry, catalysis and magnetism (Gade, 2002; Valeur & Leray, 2000; Linton & Hamilton, 1997; Saravanakumar *et al.*, 2005; Yin *et al.*, 2004). The amide linkage [–NHC(O)–] is known to be strong enough to form and maintain protein architectures and has been utilized to create various molecular devices for a spectrum of purposes in organic chemistry. We have synthesized an amide system with an aromatic ring as a terminal group to determine how the rigid ring affects the conformational behavior. In this context, we report here the molecular and crystal structure of the title compound, (I).



(I)

The asymmetric unit of (I) contains two independent molecules, as shown in Fig. 1. In both the independent molecules, the bond lengths and angles are in normal ranges (Allen *et al.*, 1987). The dihedral angle between the C3–C8 and C10–C15 benzene rings is 81.3 (2)°. The dihedral angle between the C18–C23 and C25–C30 benzene rings is 82.6 (2)°. The C3—O2—C2—C1 torsion angle is 7.4 (2)°. However, the corresponding torsion angle in the other molecule (C18—O6—C17—C16) is 83.1 (2)°.

In the crystal structure of (I), molecules are linked through intermolecular N—H···O hydrogen bonds (Table 1), forming chains running along the *b* axis (Fig. 2).

Experimental

Compound (I) was prepared according to a reported method (Zhang *et al.*, 2004). Anhydrous K_2CO_3 (0.05 mol, 7.0 g) was added slowly in portions to a dimethylformamide (DMF) solution (50 ml) of 4-nitrophenol (0.1 mmol, 13.9 g) at 383 K. An hour later, a DMF

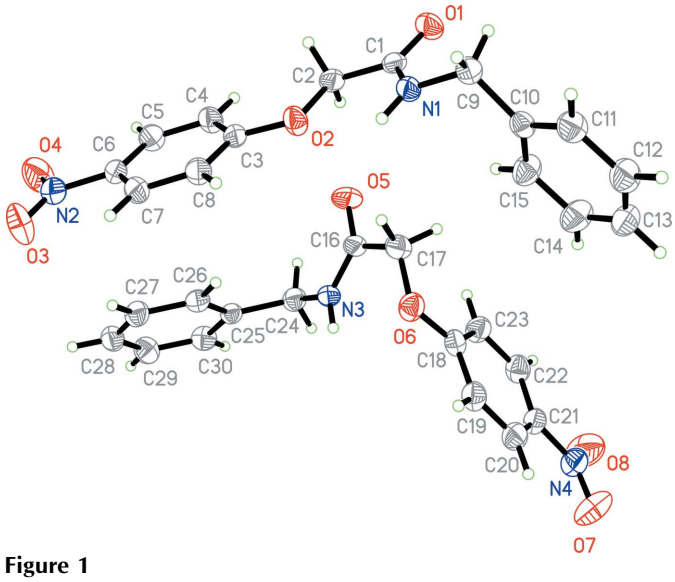


Figure 1
The asymmetric unit of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

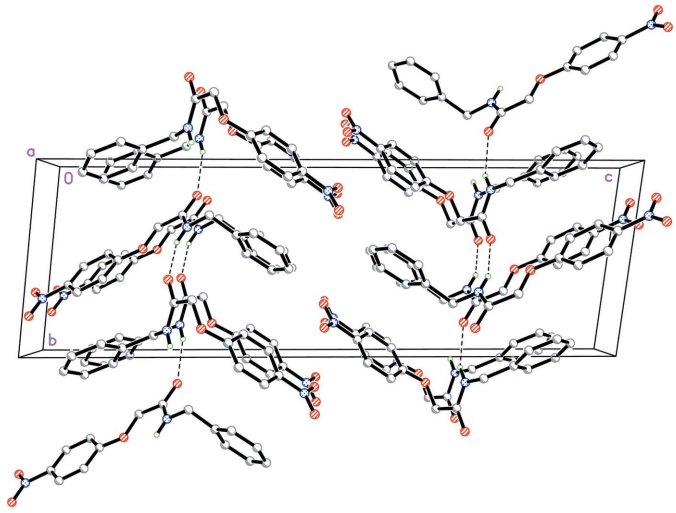


Figure 2
The molecular packing of (I). Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

solution (20 ml) containing *N*-benzyl-2-chloroacetylamide (0.1 mmol, 17.0 g) was added slowly to the mixture. The reaction mixture was stirred for 24 h at 383 K. Distilled water (50 ml) was then poured into the mixture, and the aqueous phase was extracted with $CHCl_3$. The combined organic phase was evaporated *in vacuo*. The crude product was purified by silica-gel chromatography using EtOAc–petroleum ether (1:4 *v/v*) as the eluent, affording a yellow compound. Single crystals of (I) were obtained by recrystallization from MeOH. ^{1}H NMR (200 MHz, $CDCl_3$, TMS internal reference): δ 8.38–8.41 (*t*, 1H, NH), 8.17–8.22 (*m*, 2H, *p*-NO_2–C_6H_4), 7.00–7.32 (*m*, 7H, *p*-NO_2–C_6H_4 and –C_6H_5), 4.95 (*s*, 2H, O–CH_2–CO), 4.61–4.62 (*d*, 2H, N–CH_2–Ar). Elemental analysis: found: C 62.83, H 4.88, N 9.92%; calculated: C 62.93, H 4.93, N 9.79%.

Crystal data

$C_{15}H_{14}N_2O_4$
M_r = 286.28
Triclinic, $P\overline{1}$
a = 5.821 (2) Å
b = 8.960 (3) Å
c = 26.909 (3) Å
α = 96.397 (3)°
β = 92.116 (3)°
γ = 98.070 (3)°
V = 1379.0 (7) Å^3
Z = 4
D_x = 1.379 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, yellow
0.48 × 0.46 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.953, T_{max} = 0.981
8165 measured reflections
5596 independent reflections
2885 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.130
S = 0.99
5596 reflections
380 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0164 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^{i}	0.86	2.15	2.927 (2)	150
N1—H1···O5^{ii}	0.86	2.13	2.915 (3)	151

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

H atoms were constrained to their ideal geometries, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the support of the Doctoral Research Grants of the East China University of Science and Technology (No. YJ0142119).

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.
Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Gade, L. H. (2002). *Acc. Chem. Res.* **35**, 575–582.
Linton, B. & Hamilton, A. D. (1997). *Chem. Rev.* **97**, 1669–1680.
Saravanakumar, D., Sengottuvelan, N. & Kandaswamy, M. (2005). *Inorg. Chem. Commun.* **8**, 386–389.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Valeur, B. & Leray, I. (2000). *Coord. Chem. Rev.* **205**, 3–40.
Yin, Z., Yang, Z., He, J. & Cheng, J. P. (2004). *Tetrahedron Lett.* **45**, 6803–6806.
Zhang, Y.-L., Liu, W.-S., Dou, W. & Qin, W.-W. (2004). *Spectrochim. Acta Part A*, **60**, 1707–1711.