

***N*-Ethyl-2-(4-nitrophenoxy)-*N*-phenylacetamide**Yang-Jun Ding, Guang Chen*
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The asymmetric unit of the title compound, $C_{16}H_{16}N_2O_4$, obtained from the reaction of 4-nitrophenol with *N*-ethyl-*N*-phenylchloroacetamide in dimethylformamide at 373 K, contains two crystallographically independent molecules which differ in the orientations of the ethyl groups. The dihedral angles between the two benzene rings are 57.72 (9)° and 67.78 (9)° in the two molecules.

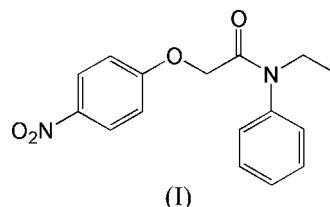
Received 16 September 2006
Accepted 16 September 2006**Key indicators**

Single-crystal X-ray study
 $T = 298$ K
 Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.051
 wR factor = 0.147
 Data-to-parameter ratio = 13.4

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

Comment

Much attention has been paid to amide-type compounds and their metal complexes for their use in molecular recognition, ion electrodes and photochemistry, their topological structure in biochemistry, catalysis, magnetics and so on (Linton & Hamilton, 1997; Lippard & Berg, 1994; Saravankumar *et al.*, 2005). The amide linkage is central to protein structure and function in biological systems (Chang *et al.*, 1991; Rebek, 1990). The amide linkage has been utilized to create various molecular devices for a variety of purposes in organic chemistry.



The title compound, (I), contains two independent molecules in the asymmetric unit (Fig. 1) which differ in the orientations of the ethyl groups [$C1-N1-C15-C16 = 95.0$ (4)° and $C17-N3-C31-C32 = -107.8$ (3)°]. The dihedral angle between the $C3-C8$ and $C9-C14$ benzene rings is 57.72 (9)° and that between the $C19-C24$ and the $C25-C30$ benzene rings is 67.78 (9)°. The corresponding bond lengths and angles in the two independent molecules agree with each other.

The crystal packing is stabilized by weak $C-H \cdots O$ interactions (Table 1).

Experimental

Compound (I) was prepared according to the literature method of Zhang *et al.* (2004). Anhydrous K_2CO_3 (4.0 g) was added slowly to a DMF solution (20 ml) of 4-nitrophenol (0.82 g) at 383 K. An hour later, a DMF solution (20 ml) containing *N*-ethyl-*N*-phenyl-2-chloroacetamide (1.18 g) was added slowly to the mixture. The reaction mixture was stirred for 24 h at 383 K. Distilled water (50 ml) was poured into the mixture, which was extracted by $CHCl_3$. The

combined organic phase was evaporated under vacuum. The crude product was chromatographed on silica gel (EtOAc/petroleum ether, 100 ml, v/v 4:1) to afford a yellow product. Single crystals of (I) were obtained by recrystallization from methanol at room temperature.

Crystal data

$C_{16}H_{16}N_2O_4$
 $M_r = 300.31$
 Triclinic, $P\bar{1}$
 $a = 9.106(2) \text{ \AA}$
 $b = 13.544(3) \text{ \AA}$
 $c = 14.530(2) \text{ \AA}$
 $\alpha = 110.318(2)^\circ$
 $\beta = 101.901(2)^\circ$
 $\gamma = 105.017(2)^\circ$

$V = 1533.9(5) \text{ \AA}^3$
 $Z = 4$
 $D_x = 1.300 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 0.10 \text{ mm}^{-1}$
 $T = 298(2) \text{ K}$
 Block, yellow
 $0.45 \times 0.40 \times 0.28 \text{ mm}$

Data collection

Siemens SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.959, T_{\max} = 0.974$

8054 measured reflections
 5318 independent reflections
 2630 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.041$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.147$
 $S = 0.96$
 5318 reflections
 397 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0605P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C2-H2B\cdots O7^i$	0.97	2.57	3.392 (4)	142
$C18-H18B\cdots O1$	0.97	2.46	3.394 (4)	161
$C23-H23\cdots O2^i$	0.93	2.42	3.335 (4)	168
$C26-H26\cdots O3^{ii}$	0.93	2.47	3.213 (5)	137

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C–H distances in the range 0.93–0.97 \AA , and with $U_{\text{iso}}(\text{H})$ set to 1.2 or 1.5 times $U_{\text{eq}}(\text{C})$.

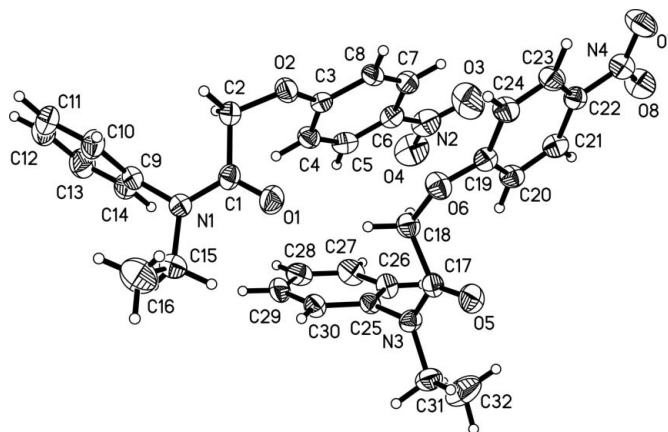


Figure 1

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

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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