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N-[2-(4-Nitrophenylamino)ethyl]acetamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.059
wR factor = 0.147
Data-to-parameter ratio = 12.4

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

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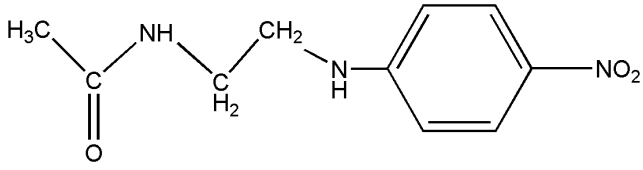
In the title compound, $C_{10}H_{13}N_3O_3$, the planar nitrophenylamine and acetamide fragments are linked in a *trans* fashion. The molecules are arranged as N—H···O hydrogen-bonded layers parallel to the (100) planes.

Comment

Imidazolinium chemistry has been intensively investigated and found to be of great utility in organic synthesis, as exemplified by the Meyers synthetic method for optically active carboxylic acids (Gant & Meyers, 1994; Kaida *et al.*, 1989). These properties stimulated our interest in this field. The title compound, (I), was obtained as an important intermediate in our synthetic investigations of imidazolinium compounds.



(I)

The title molecule contains two planar fragments linked by the C7—C8 bond in a *trans* fashion (Fig. 1); the r.m.s deviation in the nitrophenylamine fragment (C1–C7/N1/N2/O1/O2) is 0.064 Å, while that in the acetamide (C8–C10/N3/O3) fragment is 0.013 Å. The dihedral angle between these two planes is 10.66 (5)°. As shown in Fig. 2, N—H···O hydrogen bonds (Table 2) link the molecules into a layered structure parallel to the (100) planes.

Experimental

The title compound was prepared according to the method of Colapietro *et al.* (1982). Acetic anhydride (1 mmol) was added dropwise to

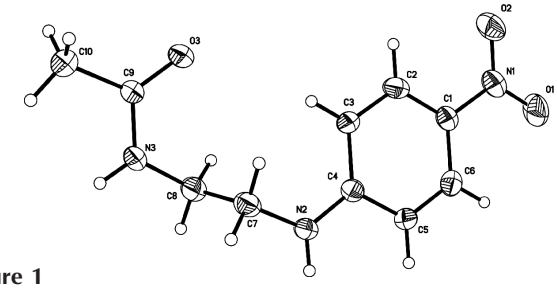


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering. H atoms are shown as small spheres of arbitrary radii.

a solution of *N*-(*p*-nitrophenyl)ethylenediamine (1 mmol) in dry ethyl alcohol (50 ml) cooled in an ice-water bath and the reaction mixture was stirred for 1 h at room temperature. A yellow precipitate was collected by filtration and recrystallized from ethyl alcohol. The product was dissolved in methanol and the solution was kept at room temperature. Yellow block-shaped crystals appeared after two weeks by slow evaporation of the solvent.

Crystal data

$C_{10}H_{13}N_3O_3$	$Z = 2$
$M_r = 223.23$	$D_x = 1.392$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 6.731$ (3) Å	Cell parameters from 716 reflections
$b = 6.882$ (3) Å	$\theta = 3.0$–$25.9°$
$c = 11.508$ (5) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 88.620$ (6)°	$T = 293$ (2) K
$\beta = 89.988$ (5)°	Block, yellow
$\gamma = 88.106$ (6)°	0.4 × 0.2 × 0.2 mm
$V = 532.6$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	1817 independent reflections
	1258 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.014$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)	$\theta_{max} = 25.0°$
	$h = -6 \rightarrow 8$
$T_{min} = 0.959$, $T_{max} = 0.979$	$k = -6 \rightarrow 8$
2180 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.059$	$w = 1/[\sigma^2(F_o^2) + (0.072P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.147$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
1817 reflections	$\Delta\rho_{min} = -0.14$ e Å^{-3}
146 parameters	

Table 1
Selected interatomic distances (Å).

O1—N1	1.237 (3)	N2—C7	1.459 (3)
O2—N1	1.240 (3)	N3—C9	1.335 (3)
N1—C1	1.417 (3)	N3—C8	1.456 (3)
N2—C4	1.344 (3)	C9—O3	1.227 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O2^{i}	0.86	2.31	3.146 (3)	164
N2—H2···O3^{ii}	0.86	2.03	2.888 (3)	173

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

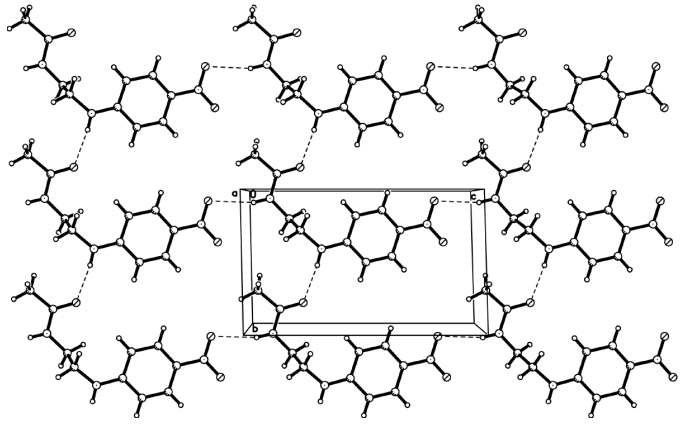


Figure 2
A view of the N—H···O hydrogen-bonded network. The hydrogen bonds are shown as dashed lines.

H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93–0.97 Å) and allowed to ride on their parent atoms, with U_{iso}(H) fixed at $1.5U_{eq}$(C) for the methylene H atoms and $1.2U_{eq}$(C,N) for other H atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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