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N-[4-(4-Nitrobenzylideneamino)phenyl]acetamide

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Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.003 Å
R factor = 0.063
wR factor = 0.142
Data-to-parameter ratio = 12.6

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

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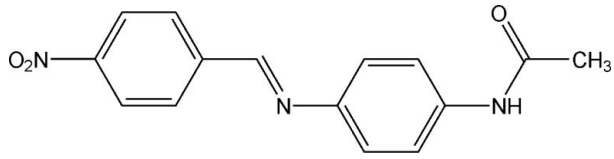
The title compund, $C_{15}H_{13}N_3O_3$, was synthesized by the solid-state reaction of 4-nitrobenzaldehyde and 4-amino-*N*-methylbenzamide. The molecules are linked head-to-tail into zigzag chains along the *c* axis by N—H···O hydrogen bonds. The molecules are further linked into sheets, parallel to (100), which are stacked in columns along [100].

Comment

The title compound, (I), was synthesized during our research into functional materials, and it showed excellent fluorescence and reversible thermochromism. To date, the title compound has not been structurally characterized and because of the structure/properties dependence, we report here its crystal structure.



(I)

The dihedral angle between the benzene ring planes is 30.1 (3)°, smaller than in published non-planar analogues (Zhang, 2002; Glidewell *et al.*, 2002). The C11—N3 distance [1.413 (3) Å] is much longer than the mean value (1.355 Å) for such bonds with N atoms having a planar configuration (Allen *et al.*, 1987).

In the crystal structure, the molecules are linked into simple chains by N—H···O hydrogen bonds (Table 1). One of the O atoms of the nitro group and the N atom of the acetamide are linked head-to-tail into chains running parallel to the *c* axis, resulting in an zigzag shape when viewed down the *a* axis (Fig. 2). In addition, these hydrogen bonds link molecules into sheets parallel to (100); these are arranged in alternating columns along the [100] direction (Fig. 3). The combination of

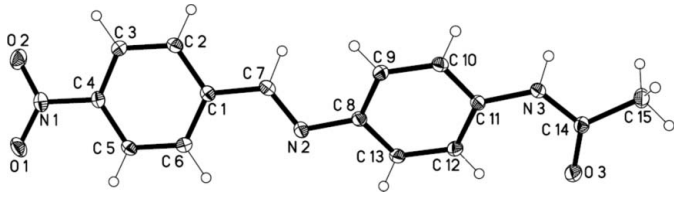


Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

the chains and the sheets generates a three-dimensional structure.

Experimental

The title compound was prepared by a conventional standard solid-state reaction technique. Equimolar quantities of 4-nitrobenzaldehyde and 4-amino-*N*-methylbenzamide were mixed and milled carefully until the mixture turned to a yellow powder. To eliminate water, the powder was kept in an oven for 1 h and was then recrystallized several times from ethanol. After a week of slow evaporation, yellow crystals of (I) formed from a chloroform–ethyl acetate (2:1) solution. Analysis found: C 63.51, H 4.67, N 14.93%; $C_{15}H_{13}N_3O_3$ requires: C 63.60, H 4.59, N 14.84%; m.p. 497–499 K.

Crystal data

$C_{15}H_{13}N_3O_3$	$Z = 8$
$M_r = 283.28$	$D_x = 1.439$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 7.0477$ (8) Å	$\mu = 0.10$ mm^{-1}
$b = 15.1868$ (17) Å	$T = 153$ (2) K
$c = 24.426$ (3) Å	Block, yellow
$V = 2614.4$ (5) Å^3	0.38 × 0.28 × 0.20 mm

Data collection

Rigaku Mercury CCD diffractometer	23604 measured reflections
ω scans	2392 independent reflections
Absorption correction: multi-scan (Jacobson, 1998)	2200 reflections with $I > 2\sigma(I)$
$T_{min} = 0.962$, $T_{max} = 0.980$	$R_{int} = 0.049$
	$\theta_{max} = 25.4°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 2.827P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.063$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.142$	$\Delta\rho_{max} = 0.45$ e Å^{-3}
$S = 1.15$	$\Delta\rho_{min} = -0.39$ e Å^{-3}
2392 reflections	
190 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3B···O1^{i}	0.88	2.43	3.263 (3)	157

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

All H atoms were positioned geometrically and refined with a riding model, with C—H distances of 0.95 Å (Csp^2), 0.98 Å (methyl) and N—H 0.88 Å, and with U_{iso}(H) values set equal to 1.5 or 1.2 times U_{eq}(carrier atom).

Data collection: *CrystalClear* (Rigaku, 2002); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

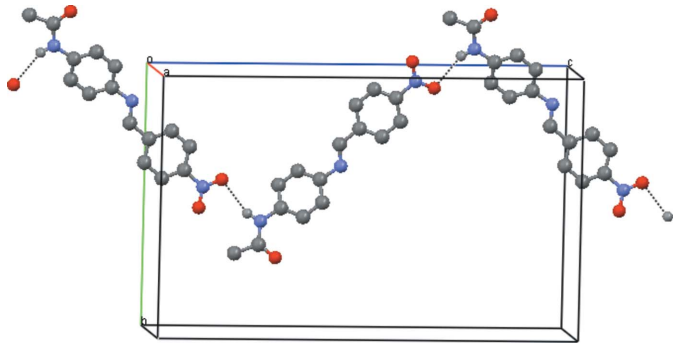


Figure 2
The zigzag hydrogen-bonded chain, viewed down the *a* axis. Dashed lines indicate hydrogen bonds. H atoms have been omitted.

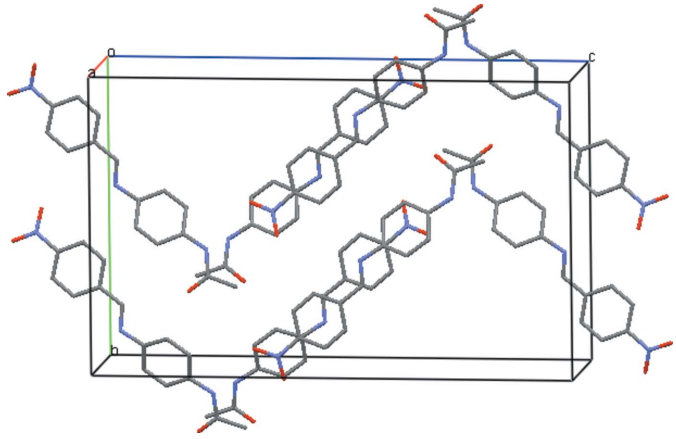


Figure 3
The molecular packing of (I) in the unit cell. H atoms have been omitted.

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