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#### Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.118  
Data-to-parameter ratio = 13.2

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

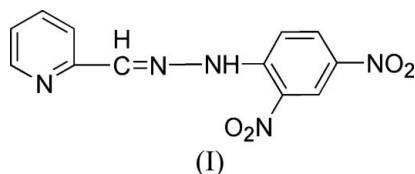
## *N*-(2,4-Dinitrophenyl)-*N'*-(2-pyridylmethylene)hydrazine

The title compound [alternative name: pyridine-2-carbaldehyde 2,4-dinitrophenylhydrazone],  $\text{C}_{12}\text{H}_9\text{N}_5\text{O}_4$ , was prepared using pyridine-2-carbaldehyde and *N*-(2,4-dinitrophenyl)hydrazine. In the crystal structure, weak intermolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen-bonding interactions link adjacent molecules to form a three-dimensional supramolecular network.

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### Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. In the present study, we report the synthesis and molecular structure of the title compound, (I).



A view of the molecule of (I) is shown in Fig. 1. In the molecular structure, the  $\text{C6}-\text{N2}$  and  $\text{N2}-\text{N3}$  bond lengths of 1.274 (2) and 1.369 (2) Å, respectively, are consistent with those found in a related structure (Jing *et al.*, 2005). The dinitrophenylhydrazone moiety and the pyridine ring are both planar, with r.m.s. deviations of the fitted atoms of 0.039 (2) and 0.005 (2) Å, respectively. The dihedral angle between the dinitrophenylhydrazone and pyridine planes is 3.88 (8)°. A strong intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond (Table 1) stabilizes the molecular conformation. In the crystal packing, two weak  $\text{C}-\text{H}\cdots\text{O}$  hydrogen-bond interactions are observed (Table 1), resulting in the formation of a three-dimensional supramolecular network.

### Experimental

An anhydrous ethanol solution of pyridine-2-carbaldehyde (1.22 g, 10 mmol) was added to an anhydrous ethanol solution of (2,4-dinitrophenyl)hydrazine (2.03 g, 10 mmol), and the mixture was stirred at 350 K for 8 h under nitrogen. The red-brown precipitate was isolated, recrystallized from ethanol, and dried *in vacuo* to give the pure compound (I) in 81% yield. Bright-red single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

## Crystal data

$C_{12}H_9N_5O_4$   
 $M_r = 287.24$   
 Monoclinic,  $P2_1/c$   
 $a = 8.5690$  (18) Å  
 $b = 6.3333$  (13) Å  
 $c = 23.340$  (5) Å  
 $\beta = 91.532$  (4)°  
 $V = 1266.2$  (5) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.507$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 1875  
 reflections  
 $\theta = 2.9$ – $25.9$ °  
 $\mu = 0.12$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 Block, red  
 $0.34 \times 0.26 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector  
 diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 1999)  
 $T_{\min} = 0.929$ ,  $T_{\max} = 0.977$   
 6807 measured reflections

2564 independent reflections  
 1567 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$   
 $\theta_{\text{max}} = 26.4$ °  
 $h = -8 \rightarrow 10$   
 $k = -7 \rightarrow 7$   
 $l = -21 \rightarrow 29$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.118$   
 $S = 0.99$   
 2564 reflections  
 194 parameters  
 H atoms treated by a mixture of  
 independent and constrained  
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.1982P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.14$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.19$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N3-H3A\cdots O1$	0.89 (1)	1.98 (2)	2.624 (2)	128 (2)
$C4-H4\cdots O4^i$	0.93	2.55	3.368 (2)	147
$C1-H1\cdots O2^{ii}$	0.93	2.54	3.402 (3)	154

Symmetry codes: (i)  $-x + 1, -y + 1, -z + 1$ ; (ii)  $-x, y + \frac{1}{2}, -z + \frac{1}{2}$

H atoms bonded to C atoms were included in calculated positions ( $C-H = 0.93$ – $0.96$  Å) and refined using a riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ . The H atom attached to N3 was located in a difference Fourier map and refined freely.

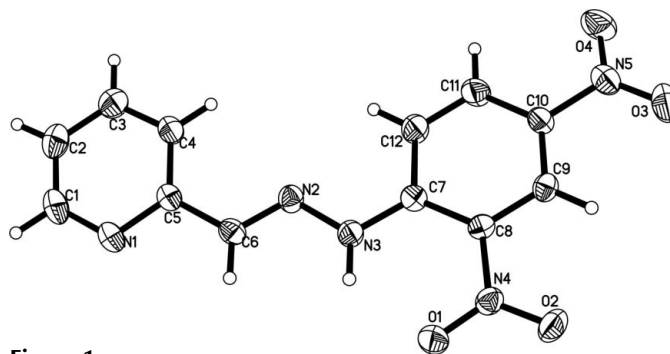


Figure 1

A view of the title compound, shown with 30% probability displacement ellipsoids.

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; 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.

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