Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(2-Furyl)-1-phenylprop-2-en-1-one 2,4-dinitrophenylhydrazone

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.044
wR factor = 0.135
Data-to-parameter ratio = 16.5

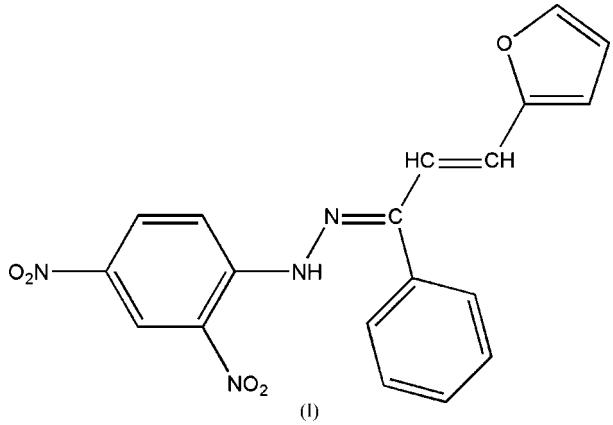
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 11 March 2006
Accepted 13 March 2006

In the title compound, $C_{19}H_{14}N_4O_5$, the dinitrophenylhydrazone and furylidene groups are nearly coplanar, making a dihedral angle of 4.50 (10)°. There is an intramolecular N—H···O hydrogen bond, while weak intermolecular C—H···O hydrogen bonds link the molecules into pseudo-dimers arranged around inversion centers.

Comment

Several phenylhydrazone derivatives have been shown to be potentially DNA-damaging and are mutagenic agents (Okabe *et al.*, 1993). One of our aims in studying Schiff bases containing nitrophenylhydrazine is to develop protein and enzyme mimics (Santos *et al.*, 2001) and obtain Schiff base structural information which will help us to investigate their coordination properties. We report here the crystal structure of the title compound, (I).



(I)

The dinitrophenylhydrazine and furylidene planes are nearly coplanar, making a dihedral angle of only 4.50 (10)°; the phenyl ring is roughly perpendicular to these planes, making dihedral angles of 85.24 (5) and 81.76 (5)°, respectively (Fig. 1).

The C1—C2 and C1—C6 bond lengths are longer than the other C—C bond lengths in the same ring, consistent with other dinitrophenyldrazone derivatives (Ohba, 1996; Bolte & Dill, 1998). An intramolecular N—H···O hydrogen bond is observed in the title compound, (I) (Fig. 1). In adition, weak intermolecular C—H···O hydrogen bonds link the molecules into pseudo-dimers arranged around inversion centers (Fig. 2).

Experimental

2,4-Dinitrophenylhydrazine (1 mmol, 0.198 g) was dissolved in anhydrous ethanol, then H_2SO_4 (98%, 0.5 ml) was added and the

mixture was stirred for several minutes at 351 K. Furylideneacetophenone (1 mmol, 0.186 g) in ethanol (6 ml) was then added dropwise and the mixture was stirred under reflux for 3 h. The product was separated and recrystallized from dichloromethane. Brown single crystals of (I) were obtained after 2 d.

Crystal data

$C_{19}H_{14}N_4O_5$
M_r = 378.34
Monoclinic, $P2_1/n$
a = 8.1605 (5) Å
b = 17.7094 (11) Å
c = 12.8041 (8) Å
β = 100.058 (1)°
V = 1822.0 (2) Å^3
Z = 4
D_x = 1.379 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4026 reflections
θ = 2.8–27.3°
μ = 0.10 mm^{-1}
T = 291 (2) K
Block, brown
0.37 × 0.30 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.963, T_{max} = 0.978
15658 measured reflections
4181 independent reflections
2780 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 27.5°
$h = -10 \rightarrow 10$
$k = -23 \rightarrow 22$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.135
S = 1.05
4181 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.2674P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1	0.86	1.96	2.6014 (18)	131
C13—H13···O4^{i}	0.93	2.35	3.276 (2)	176

Symmetry code: (i) $-x+1, -y+1, -z+1$.

All H atoms were introduced in calculated positions and treated as riding on their parent atoms, with N—H = 0.86 Å and C—H = 0.93 Å, with U_{iso}(H) = 1.2U_{eq}(N,C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors express their deep appreciation to the Startup Fund for PhDs of the Natural Scientific Research of Zhengzhou University of Light Industry (No. 2005001) and the Startup Fund for Masters of the Natural Scientific Research of Zhengzhou University of Light Industry (No. 000455).

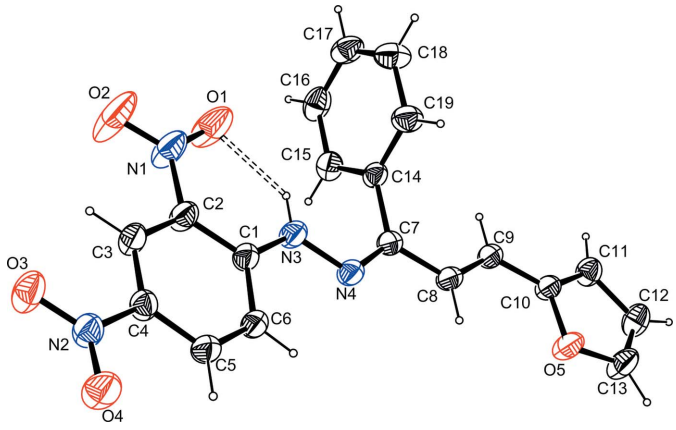


Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates the intramolecular hydrogen bond and H atoms are shown as small spheres of arbitrary radii.

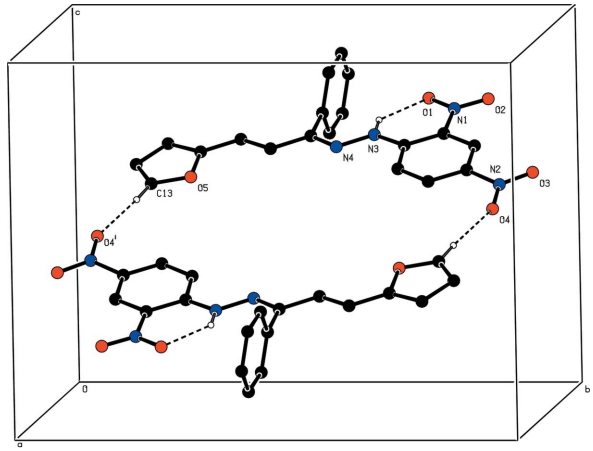


Figure 2
View showing the weak intermolecular C—H···O hydrogen bonds (dashed lines) linking two molecules around an inversion center. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

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