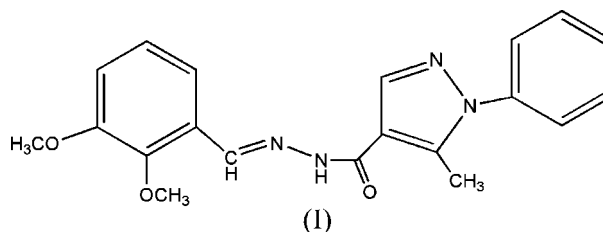


***N'*-(2,3-Dimethoxybenzylidene)-5-methyl-1-phenyl-1*H*-pyrazole-4-carbohydrazide**Shu-Wen Wang,^a Li-Rong Wen^{a*}
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Key indicatorsSingle-crystal X-ray study
T = 294 K
Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
R factor = 0.053
wR factor = 0.149
Data-to-parameter ratio = 13.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.The crystal packing of the title compound, $\text{C}_{20}\text{H}_{20}\text{N}_4\text{O}_3$, is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{N}$ hydrogen-bond interactions.Received 27 June 2006
Accepted 18 July 2006**Comment**As special Schiff bases, acylhydrazones have been extensively investigated because of their strong tendency to chelate transition metals (Naskar *et al.*, 2004) and their pharmacological applications (Sreekanth *et al.*, 2004). A number of acylhydrazones and their transition metal complexes have been reported to inhibit biological activity and have been used as anti-inflammatory, sterilization and antitumour agents (Buu-Hoi *et al.*, 1953). In this paper, we report the crystal structure of the title acylhydrazone derivative, (I), which was obtained by reaction of pyrazolyhydrazone with dimethoxybenzaldehyde.

Bond lengths and angles in (I) are as expected for this type of compound. The pyrazole ring is planar, with a maximum deviation of 0.012 (3) Å for atom N1, and forms a dihedral angle of 64.80 (12)° with the plane of the C1–C6 benzene ring. The carbonyl group is synperiplanar to the pyrazole ring double bond with a C8–C9–C11–O1 torsion angle of 10.9 (7)°.

In the crystal structure, molecules are linked into centrosymmetric dimers through intermolecular $\text{N}-\text{H}\cdots\text{O}$ interactions (Table 1), which form six-membered rings. In addition, the crystal packing is stabilized by weak intermolecular $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds (Table 1 and Fig. 2) and $\text{C}-\text{H}\cdots\pi$ interactions [$\text{C}5-\text{H}5\cdots\text{C}g1^{\text{iii}} = 2.71 \text{ \AA}$; $\text{C}15-\text{H}15\cdots\text{C}g2^{\text{iv}} = 2.94 \text{ \AA}$; *Cg*1 and *Cg*2 are the centroids of the C13–C18 and C1–C6 benzene rings, respectively; symmetry codes: (iii) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (iv) $-x, -\frac{1}{2} + y, \frac{1}{2} + z$].**Experimental**A mixture of 5-methyl-1-phenyl-4-pyrazolhydrazone (2 mmol), synthesized according to the literature method (Li *et al.*, 2004), 2,3-dimethoxybenzaldehyde (2 mmol) and anhydrous ethanol (10 ml) was stirred in a 100 ml flask for 4 h at room temperature. The

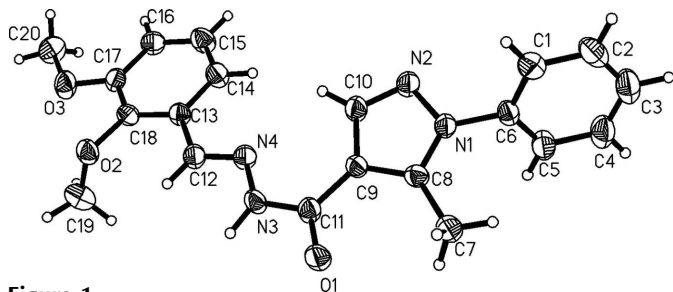


Figure 1
The molecular structure of the title compound, with 35% probability displacement ellipsoids.

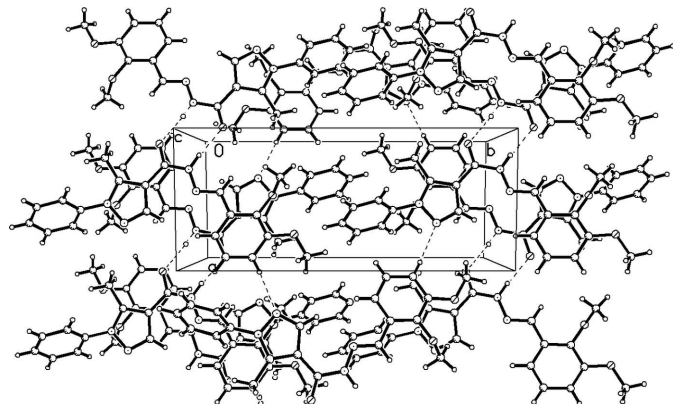


Figure 2
The molecular packing of the title compound, viewed along the *c* axis. Intermolecular hydrogen bonds are shown as dashed lines.

progress of the reaction was monitored by thin layer chromatography. After completion of the reaction, the mixture was filtered to obtain the crude product. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution (m.p. 461 K).

Crystal data

$C_{20}H_{20}N_4O_3$
 $M_r = 364.40$
Monoclinic, $P2_1/c$
 $a = 6.962$ (2) Å
 $b = 16.343$ (5) Å
 $c = 16.934$ (5) Å
 $\beta = 101.803$ (6)°
 $V = 1886.0$ (10) Å³

$Z = 4$
 $D_x = 1.283$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 294$ (2) K
Prism, colourless
 $0.24 \times 0.22 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.973$, $T_{\max} = 0.983$

6595 measured reflections
3330 independent reflections
1457 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.057$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.149$
 $S = 0.99$
3330 reflections
251 parameters
H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.4319P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N3—H3A...O1 ⁱ	0.91 (4)	1.93 (4)	2.841 (4)	175 (4)
C16—H16...N2 ⁱⁱ	0.93	2.57	3.499 (6)	176

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

The H atom attached to N3 was located in a difference Fourier synthesis and its positional parameters were refined, with the N—H distance restrained to 0.91 (2) Å. All other H atoms were placed in calculated positions, with C—H = 0.93–0.96 Å and included in the final cycles of refinement using a riding model. The isotropic displacement parameters of all H atoms were fixed at 1.2 or 1.5 times U_{eq} of the parent atoms.

Data collection: SMART (Bruker, 1998); 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, 1999); software used to prepare material for publication: SHELXTL.

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