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(*E*)-4-(6-Methoxy-2-naphthylmethylideneamino)-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

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In the title compoumd, $C_{23}H_{21}N_3O_2$, all the bond lengths and angles have normal values. The naphthalene ring system and the pyrazole ring are approximately coplanar and are linked by an HC=N unit, forming a conjugated system. In the crystal structure, weak C—H···O interactions link the molecules, forming a layer structure.

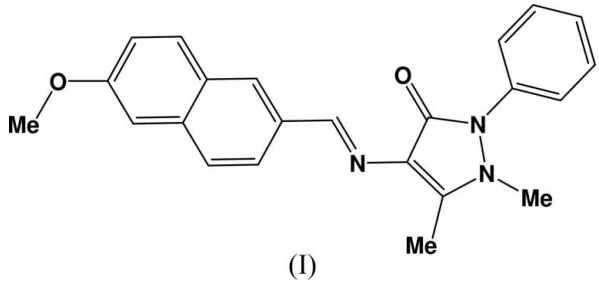
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.076
Data-to-parameter ratio = 14.6

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

Comment

Some Schiff base ligands and their transition metal complexes have been used as models for biological systems (Costamagna *et al.*, 1992; Chen & Martell, 1987), catalysts for some organic reactions (Canail & Sherrington, 1999) and non-linear optical materials (Alemi & Shaabani, 2000). In order to study the relationship between the structure and properties of this kind of compound, some Schiff base compounds containing a phenazone scaffold were recently synthesized (Yang *et al.*, 2006; Zheng *et al.*, 2006). As a continuation of this research, the title compound, (I), a new derivative of this kind, was synthesized and its structure is presented here.



(I)

The molecular structure is shown in Fig. 1. All bond lengths and angles have normal values. The N1—N2 distance is 1.4068 (16) Å, which is typical for a single bond. The naphthalene ring system and the pyrazole ring are approximately coplanar, with a dihedral angle of 7.39 (7)°, and are linked by an HC=N unit, forming a conjugated system. In the crystal structure, weak C—H···O interactions link the molecules, forming a layer structure (Table 1 and Fig. 2).

Experimental

Under nitrogen, 4-aminophenazone (2.03 g, 10 mmol) was added to an ethanol solution (25 ml) of 6-methoxynaphthaldehyde (1.86 g, 10 mmol); the resulting mixture was refluxed for 6 h, yielding a yellow precipitate. The product was collected *via* vacuum filtration and washed with ethanol. The crude product was recrystallized from a mixture of ethanol and *n*-hexane (1:4) and yellow crystals were obtained in 86% yield.

Crystal data

$C_{23}H_{21}N_3O_2$
M_r = 371.43
Monoclinic, $P2_1/n$
a = 8.102 (2) Å
b = 7.1317 (19) Å
c = 33.558 (9) Å
β = 90.761 (4)°
V = 1938.9 (9) Å^3
Z = 4
D_x = 1.272 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 273 (2) K
Block, yellow
0.30 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: none
11973 measured reflections
3742 independent reflections
1910 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.076
S = 1.00
3742 reflections
256 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O1^{i}	0.96	2.45	3.371 (2)	161
C9—H9···O2^{ii}	0.93	2.60	3.346 (2)	137

Symmetry codes: (i) $x, y-1, z$; (ii) $x+\frac{1}{2}, -y+\frac{5}{2}, z+\frac{1}{2}$.

H atoms were positioned geometrically, with C—H = 0.93–0.96 Å, and included in the refinement as riding, with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Mercury* (Version 1.4.1; Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL*.

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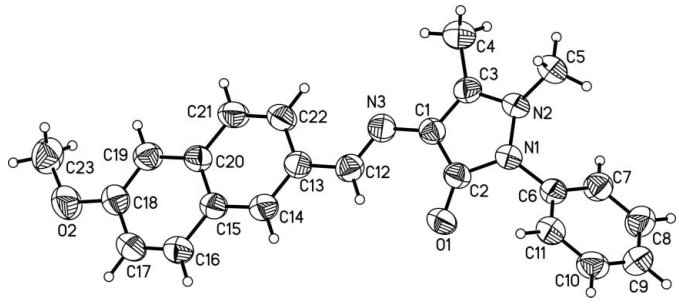

Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

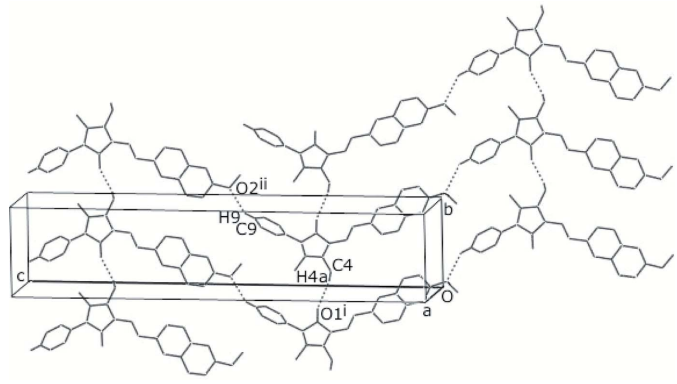

Figure 2
View of the layer structure generated by hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (i) $x, y-1, z$; (ii) $\frac{1}{2}+x, \frac{5}{2}-y, \frac{1}{2}+z$.]

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