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4-[(*Z*)-(4-Methoxyanilino)phenylmethylene]-5-methyl-2-phenyl-2*H*-pyrazol-3(4*H*)-one

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The crystal structure of the title compound, $C_{24}H_{21}N_3O_2$, features a central pyrazole ring; the NH unit interacts with the C=O unit through an intramolecular hydrogen bond [N···O = 2.714 (1) Å].

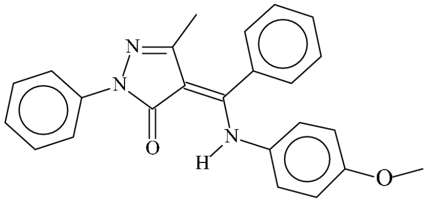
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.124
Data-to-parameter ratio = 16.2

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

Comment

This study is a continuation of our study of 4-[(*Z*)-(2-arylamino)phenylmethylene]-5-methyl-2-phenyl-2*H*-pyrazol-3-ones, which are readily synthesized by condensing 4-benzoyl-3-methyl-1-phenyl-5-pyrazolone with a primary amine (Bao, Lü, Wu, Kang & Ng, 2004; Bao, Lü, Wu, & Ng, 2004; Jiang *et al.*, 2004). A characteristic of such pyrazolones is the short intramolecular hydrogen bond between the amino NH unit and the carbonyl C=O unit; the nature of the organic group connected to the amino group does not appear to have a significant effect on the bond unless the group itself possesses sites that are capable of other interactions. The 4-methoxyphenyl derivative, (I) (Fig. 1), similarly exists as a monomeric molecule that features an intramolecular hydrogen bond [2.714 (1) Å].



(I)

Experimental

4-Benzoyl-3-methyl-1-phenyl-5-pyrazolone (2.20 g, 7.9 mmol) and *p*-methoxyaniline (0.99 g, 8.0 mmol) were dissolved in formic acid (35 ml). The solution was heated under reflux for 8 h. The solvent was removed and the pure product obtained upon recrystallization from a 1:1 ethanol/*n*-heptane mixture (45 ml) in about 80% yield. Crystals were grown from ethanol. Analysis calculated for $C_{24}H_{21}N_3O_2$: C 75.20, H 5.48, N 10.97%; found: C 75.30, H 5.39, N 10.68%.

Crystal data

$C_{24}H_{21}N_3O_2$	$Z = 2$
$M_r = 383.44$	$D_x = 1.261$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 6.8262$ (9) Å	Cell parameters from 904 reflections
$b = 10.951$ (1) Å	$\theta = 2.0$–$27.1°$
$c = 14.761$ (1) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 97.259$ (2)°	$T = 298$ (2) K
$\beta = 103.386$ (2)°	Block, yellow
$\gamma = 106.018$ (2)°	0.50 × 0.50 × 0.20 mm
$V = 1010.2$ (2) Å^3	

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: none
8643 measured reflections
4350 independent reflections
3303 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.013$
$\theta_{\rm max} = 27.1°$
$h = -8 \rightarrow 8$
$k = -13 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.124$
$S = 1.01$
4350 reflections
268 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0692P)^2 + 0.1202P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.15$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.244 (2)	C7—C8	1.444 (2)
N1—N2	1.397 (2)	C8—C11	1.391 (2)
N1—C7	1.376 (2)	C8—C9	1.433 (2)
N1—C1	1.414 (2)	C9—C10	1.490 (2)
N2—C9	1.303 (2)		
N2—N1—C1	118.7 (1)	C7—C8—C9	105.2 (1)
N2—N1—C7	112.2 (1)	C7—C8—C11	122.2 (1)
C1—N1—C7	128.5 (1)	C9—C8—C11	132.2 (1)
C9—N2—N1	106.4 (1)	N2—C9—C8	111.7 (1)
O1—C7—N1	126.2 (1)	N2—C9—C10	118.5 (1)
N1—C7—C8	104.4 (1)	C8—C9—C10	129.8 (1)
O1—C7—C8	129.3 (1)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*n*···O1	0.87 (1)	1.96 (1)	2.714 (1)	145 (2)

The H atoms were placed at calculated positions [C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for the aromatic H atoms and C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for the methyl H atoms] and included in the refinement in the riding-model approximation. The amino H atom was located and refined with an N—H distance restraint of 0.85 (1) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

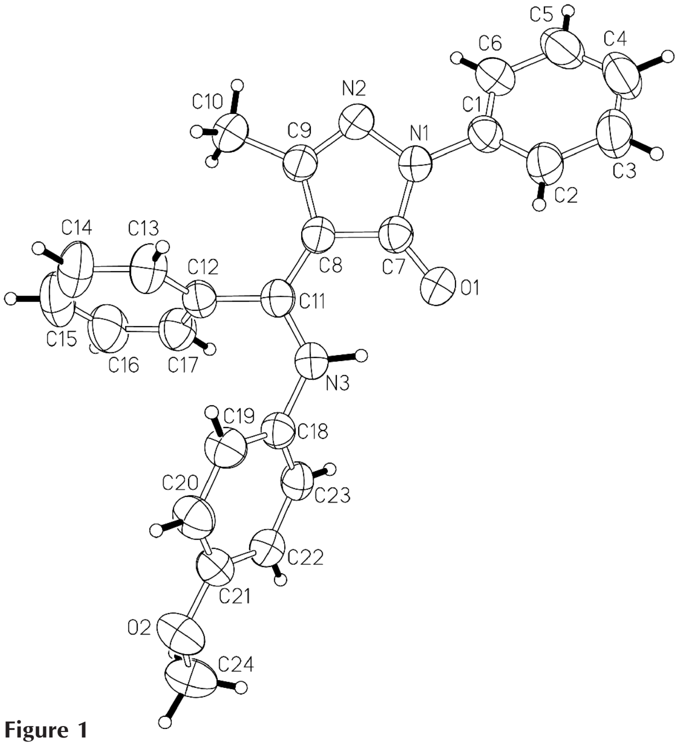


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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