Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Methyl-1-phenyl-4-[(*Z*)-phenyl(*p*-tolylamino)-methylene]-1*H*-pyrazol-5(4*H*)-one

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Received 18 July 2005
Accepted 19 August 2005
Online 17 September 2005

Key indicators

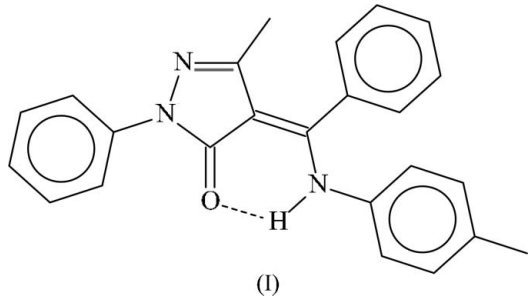
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.121
Data-to-parameter ratio = 14.7

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

The NH unit on the exocyclic C=C double bond in the title compound, $C_{24}H_{21}N_3O$, which is on the same side of the double bond as the C=O unit of the pyrazolone ring, interacts with the carbonyl group through an intramolecular N—H···O hydrogen bond [2.685 (2) Å].

Comment

5-Methyl-2-phenyl-4-[(*Z*)-(2-tolylamino)phenylmethylene]-pyrazol-3(2*H*)-one exists as a monomeric compound whose NH unit is linked to the C=O unit by a short [N···O = 2.695 (2) Å] hydrogen bond (Bao *et al.*, 2004). The isomeric title compound, (I) (Fig. 1), displays a somewhat shorter hydrogen bond [2.685 (2) Å]; otherwise, there are no significant differences between the two isomers. The two hydrogen bonds are slightly shorter than that found in 4-[(phenyl)phenylmethylene]-5-methyl-2-phenyl-2*H*-pyrazol-3-one [2.704 (2) Å; Ma, 2005].



(I)

Experimental

1-Phenyl-3-methyl-4-benzoyl-5-pyrazolone (2.50 g, 9.0 mmol) and 4-aminotoluene (0.96 ml, 9.4 mmol) were dissolved in ethanol (35 ml) and the solution was refluxed for 6 h. The solvent was removed and the pure title compound was obtained upon recrystallization from a 1:1 ethanol/*n*-heptane mixture (35 ml) in about 75% yield. Crystals were grown from an ethanol solution. Analysis calculated for $C_{24}H_{21}N_3O$: C 78.45, H 5.76, N 11.44%; found: C 78.37, H 5.42, N 11.61%.

Crystal data

$C_{24}H_{21}N_3O$
M_r = 367.44
Triclinic, $P\overline{1}$
a = 7.4272 (10) Å
b = 11.0766 (14) Å
c = 13.6124 (17) Å
α = 110.095 (2)°
β = 99.798 (2)°
γ = 104.067 (2)°
V = 979.8 (2) Å^3
Z = 2
D_x = 1.245 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 892 reflections
θ = 2.1–26.1°
μ = 0.08 mm^{-1}
T = 295 (2) K
Block, yellow
0.50 × 0.45 × 0.27 mm

Data collection

Bruker SMART area-detector diffractometer	$R_{int} = 0.013$
ω scans	$\theta_{max} = 26.1^\circ$
5537 measured reflections	$h = -9 \rightarrow 9$
3811 independent reflections	$k = -10 \rightarrow 13$
2816 reflections with $I > 2\sigma(I)$	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0638P)^2 + 0.1375P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.121$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.15$ e Å^{-3}
3811 reflections	
259 parameters	
H atoms treated by a mixture of independent and constrained refinement	

The C-bound H atoms were positioned geometrically [C—$H_{aromatic}$ = 0.93 Å and Uiso(H) = 1.2U_{eq}(C); C—H_{methyl} = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C)], and were included in the refinement in the riding model approximation; the methyl groups were rotated for a best fit with the electron density. The N-bound H atom was located in a difference Fourier map and was refined with a distance restraint of N—H = 0.86 (1) Å. The displacement parameter of this H atom was also refined.

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: *ORTEP* in *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXL97*.

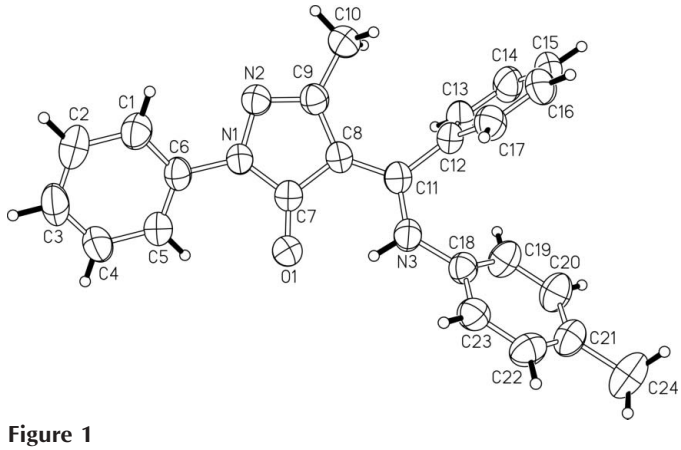


Figure 1
ORTEP (Bruker, 1999) plot showing the numbering scheme of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii.

The author thanks Xianning College for supporting this study.

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