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4-[(*Z*)-(2,4-Dimethylphenylamino)phenylmethylene]-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one

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The NH unit on the exocyclic C=C double bond in the title compound, $C_{25}H_{23}N_3O$, interacts with the carbonyl group through an intramolecular hydrogen bond.

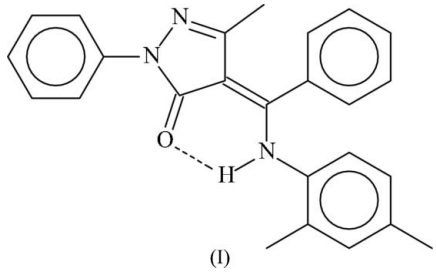
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.054
wR factor = 0.130
Data-to-parameter ratio = 17.5

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

Comment

The title compound, (I) (Fig. 1) has two methyl substituents in the 2,4-dimethylphenylamino portion of the molecule; the general features are similar to those found in the analogous 2-tolylamino (Bao *et al.*, 2004) and 4-tolylamino (Ma, 2005) derivatives. The compound is used to chelate to a divalent transition metal (Ma *et al.*, 2006).



(I)

Experimental

1-Phenyl-3-methyl-4-benzoyl-5-pyrazolone (1.60 g, 5.8 mm mol) and 2,4-dimethylaniline (0.73 g, 6.0 mm mol) were dissolved in ethanol (35 ml); formic acid (0.5 ml) was added to catalyse the reaction. 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 in 80% yield. Crystals were grown from an ethanol solution of the compound. Elemental analysis calculated for $C_{25}H_{23}N_3O$: C 79.29, H 9.15, N 11.56%; found: C 79.10, H 9.26, N 11.27%.

Crystal data

$C_{25}H_{23}N_3O$
M_r = 381.46
Triclinic, $P\overline{1}$
a = 7.909 (1) Å
b = 11.200 (1) Å
c = 13.239 (1) Å
α = 106.410 (2)°
β = 106.327 (2)°
γ = 100.390 (2)°
V = 1035.6 (2) Å^3
Z = 2
D_x = 1.223 Mg m^{-3}
Mo *Kα* radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
Block, yellow
0.10 × 0.06 × 0.04 mm

Data collection

Bruker APEX area-detector diffractometer
ω and φ scans
Absorption correction: none
10060 measured reflections
4633 independent reflections
2018 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 27.5°

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.047P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.130$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.83$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
4633 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
265 parameters	

H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [phenyl C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C); methyl C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C)]; the methyl groups were rotated to fit the electron density. The amino H atom was similarly constrained [N—H = 0.86 Å and U_{iso}H = 1.2U_{eq}(N)].

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

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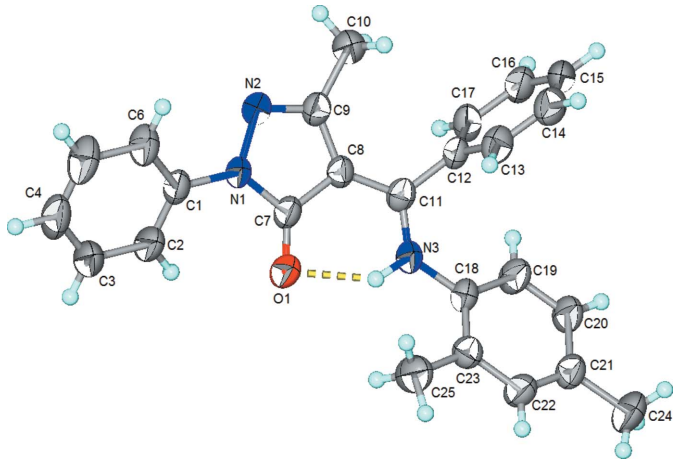

Figure 1
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. The dashed line denotes the intramolecular hydrogen bond.

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