

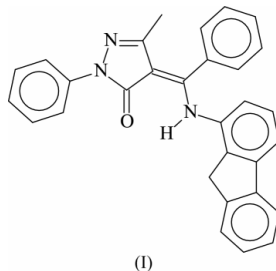
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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.042
 wR factor = 0.116
Data-to-parameter ratio = 16.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.4-[(*Z*)-(2-Fluorenylamino)phenylmethylene]-
5-methyl-2-phenyl-2*H*-pyrazol-3(4*H*)-oneThe NH unit on the exocyclic C=C double bond in the title
compound, $\text{C}_{30}\text{H}_{23}\text{N}_3\text{O}$, lies on the same side of the double
bond as the carbonyl unit of the pyrazolonyl ring, and the two
interact through an $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond [2.671 (2) Å].

Comment

Two earlier studies reported on 4-[(*Z*)-(2-arylamino)phenyl-
methylene]-5-methyl-2-phenyl-2*H*-pyrazol-3-ones (Bao *et al.*,
2004; Jiang *et al.*, 2004), a class of pyrazolones that are readily
synthesized from a benzoylpyrazolone and a primary amine.
For the present study, the primary amine selected for the
condensation was 2-aminofluorene; the amine itself features
 $\text{N}-\text{H}\cdots\pi$ hydrogen-bonding interactions in the solid state
(Steiner, 2000). The title compound, (I) (Fig. 1) shows struc-
tural features that are similar to those in reported compounds,
such as, for example, a short intramolecular amino-carbonyl
hydrogen bond.

Experimental

1-Phenyl-3-methyl-4-benzoyl-5-pyrazolone (3.20 g, 11.5 mmol) and
2-aminofluorene (2.26 g, 12.5 mmol) were dissolved in ethanol
(35 ml); formic acid (0.5 ml) was added to catalyse the reaction. The
solution was heated under reflux for several hours. The solvent was
removed and the pure product obtained upon recrystallization from a
1:1 ethanol/*n*-heptane mixture in 85% yield. Crystals were grown
from an ethanol solution. Elemental analysis calculated for
 $\text{C}_{30}\text{H}_{23}\text{N}_3\text{O}$: C 81.61, H 5.25, N 9.52%; found: C 81.90, H 5.36, N
9.38%.

Crystal data

 $\text{C}_{30}\text{H}_{23}\text{N}_3\text{O}$
 $M_r = 441.51$
Monoclinic, $P2_1/n$
 $a = 9.700$ (1) Å
 $b = 22.441$ (3) Å
 $c = 10.638$ (1) Å
 $\beta = 94.583$ (3)°
 $V = 2308.4$ (5) Å³
 $Z = 4$ $D_x = 1.270$ Mg m⁻³
Mo $K\alpha$ radiation
Cell parameters from 934
reflections
 $\theta = 2.9$ – 25.7 °
 $\mu = 0.08$ mm⁻¹
 $T = 298$ (2) K
Block, colorless
 $0.37 \times 0.30 \times 0.23$ mm

Data collection

Bruker SMART area-detector
diffractometer
 φ and ω scans
Absorption correction: none
13811 measured reflections
5038 independent reflections

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.116$
 $S = 1.00$
5038 reflections
312 parameters
H atoms treated by a mixture of
independent and constrained
refinement

2835 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$
 $\theta_{\text{max}} = 27.0^\circ$
 $h = -12 \rightarrow 10$
 $k = -28 \rightarrow 28$
 $l = -11 \rightarrow 13$

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.2453P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.16 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.15 \text{ e } \text{\AA}^{-3}$

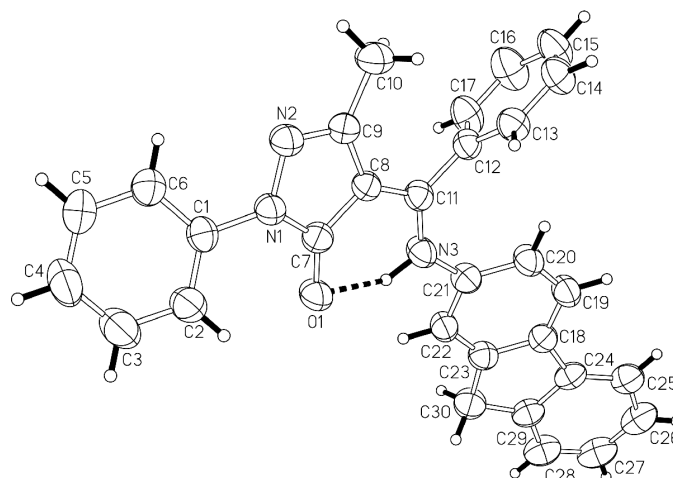


Figure 1

An ORTEPII (Johnson, 1976) plot of (I) at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

$H = 0.96 \text{ \AA}$ for the methyl H atoms and $C-H = 0.97 \text{ \AA}$ for the methylene H atoms), and their displacement parameters were set to 1.2 times U_{eq} of the parent atoms for the aromatic and methyl C atoms, and to 1.5 times U_{eq} for the methyl C atom. The methyl group was allowed to rotate but not to tip. The amino H atom was located and refined.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Table 1

Selected geometric parameters (\AA , $^\circ$).

O1–C7	1.251 (2)	C18–C24	1.471 (2)
N1–C7	1.375 (2)	C19–C20	1.377 (2)
N1–N2	1.404 (2)	C20–C21	1.392 (2)
N1–C1	1.420 (2)	C21–C22	1.392 (2)
N2–C9	1.308 (2)	C22–C23	1.382 (2)
N3–C11	1.339 (2)	C23–C30	1.503 (2)
N3–C21	1.417 (2)	C24–C25	1.385 (2)
C7–C8	1.441 (2)	C24–C29	1.399 (2)
C8–C11	1.397 (2)	C25–C26	1.391 (3)
C8–C9	1.429 (2)	C26–C27	1.380 (3)
C9–C10	1.496 (2)	C27–C28	1.380 (3)
C11–C12	1.483 (2)	C28–C29	1.376 (2)
C18–C19	1.384 (2)	C29–C30	1.509 (2)
C18–C23	1.392 (2)		
C7–N1–N2	111.6 (1)	C23–C18–C24	108.2 (2)
C7–N1–C1	128.1 (1)	C20–C19–C18	119.7 (2)
N2–N1–C1	118.8 (1)	C19–C20–C21	120.5 (2)
C9–N2–N1	106.4 (1)	C22–C21–C20	119.9 (2)
C11–N3–C21	133.0 (2)	C22–C21–N3	114.8 (2)
C6–C1–N1	119.6 (2)	C20–C21–N3	125.2 (2)
C2–C1–N1	120.7 (2)	C23–C22–C21	119.5 (2)
O1–C7–N1	125.9 (2)	C22–C23–C18	120.2 (2)
N1–C7–C8	105.0 (1)	C22–C23–C30	129.2 (2)
C11–C8–C9	132.5 (2)	C18–C23–C30	110.6 (2)
C11–C8–C7	122.3 (2)	C25–C24–C29	120.3 (2)
C9–C8–C7	105.2 (1)	C25–C24–C18	131.1 (2)
N2–C9–C8	111.8 (1)	C29–C24–C18	108.6 (2)
N2–C9–C10	118.4 (2)	C24–C25–C26	118.6 (2)
C8–C9–C10	129.8 (2)	C27–C26–C25	120.7 (2)
N3–C11–C8	117.2 (2)	C26–C27–C28	120.7 (2)
N3–C11–C12	121.0 (1)	C29–C28–C27	119.2 (2)
C8–C11–C12	121.8 (2)	C28–C29–C24	120.4 (2)
C17–C12–C11	120.7 (2)	C28–C29–C30	129.7 (2)
C13–C12–C11	119.7 (2)	C24–C29–C30	109.9 (2)
C19–C18–C23	120.2 (2)	C23–C30–C29	102.7 (1)
C19–C18–C24	131.6 (2)		

The H atoms were placed at calculated positions in the riding-model approximation ($C-H = 0.93 \text{ \AA}$ for the aromatic H atoms, $C-$