

Hai-Zhen Xu,^{a*} Xue-Kai Si,^b
You-Quan Zhu^b and Hai-Bin
Song^b^aCollege of Chemistry and Life Science, Tianjin Normal University, Weijin Road No. 241, Tianjin, People's Republic of China, and ^bState Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, People's Republic of ChinaCorrespondence e-mail:
zyq8165@nankai.edu.cn

Key indicators

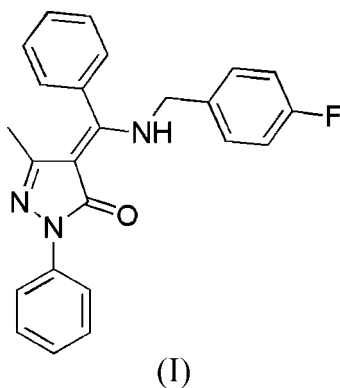
Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(C-C) = 0.006$ Å
 R factor = 0.056
 wR factor = 0.168
Data-to-parameter ratio = 13.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(4Z)-4-[(4-Fluorobenzylamino)(phenyl)-methylene]-3-methyl-1-phenyl-1H-pyrazol-5(4H)-one**

In the title compound, $C_{24}H_{20}FN_3O$, the dihedral angles formed by the pyrazolone ring with the three benzene rings are 10.45 (7), 89.05 (12) and 83.90 (12)°. The compound is a ligand in an enamine-keto form and its structure is stabilized by three intramolecular N—H···O hydrogen bonds. Glide-related molecules form C—H···O hydrogen-bonded chains along the b axis.

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Comment

1-Phenyl-3-methyl-4-benzoylpyrazolon-5-one (HPMBP), an effective β -diketonate, is widely used and well known for its extractive ability. In recent years, it and its metal complexes have also been found to have good antibacterial and biological properties. Its metal complexes have analgesic activity (Liu *et al.*, 1980; Li *et al.*, 1997; Zhou *et al.*, 1999). Organic fluorine compounds have received significant attention in the materials and pharmaceutical sciences due to their unique physical and biological properties, such as increased membrane permeability, enhanced hydrophobic binding and stability against metabolic oxidation (Kirsch, 2004; Ojima *et al.*, 1996). In order to develop new medicines, we have synthesized the title compound, (I), and its structure is reported here.



The structure of (I) is shown in Fig. 1. The pyrazolone ring is nearly coplanar with the C1–C6 benzene ring and nearly perpendicular to the other two benzene rings (C12–C17 and C19–C24); the dihedral angles are 10.45 (7), 89.05 (12) and 83.90 (12)°, respectively. The O atom of the 3-methyl-1-phenylpyrazol-5-one unit and the N atom of the (4-fluorophenyl)methanamine group are available for coordination with metals. The pyrazolone ring is planar and atoms O1, C7, C8, C11 and N3 are coplanar, the largest deviation being 0.0154 (20) Å for atom C7. The dihedral angle between this

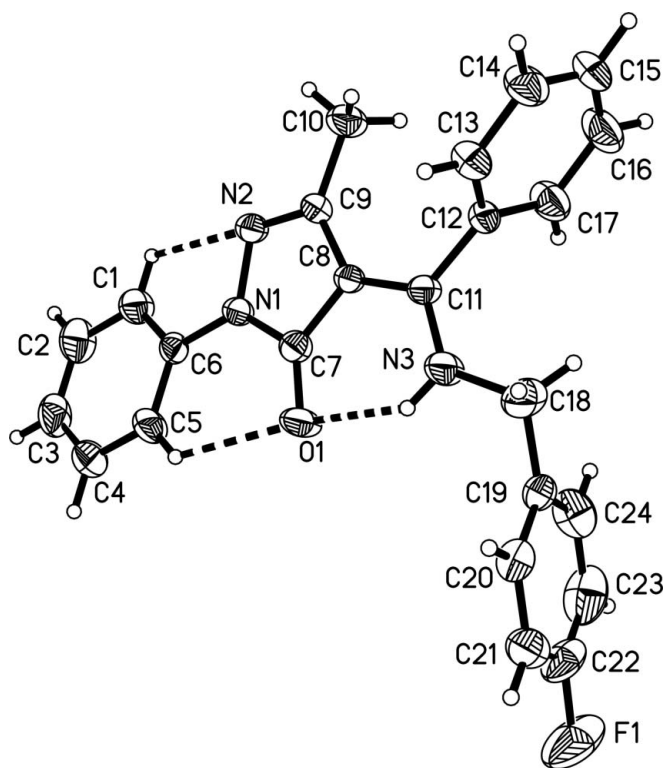


Figure 1
A view of (I), with displacement ellipsoids drawn at the 50% probability level. Dashed lines indicate hydrogen bonds.

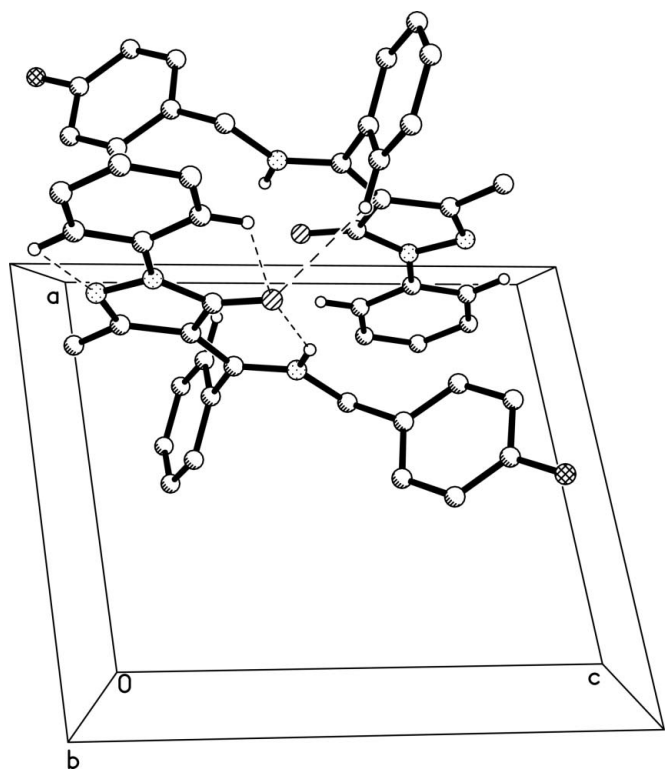


Figure 2
Intra- and intermolecular hydrogen bonds (dashed lines) in the structure of (I).

mean plane and the pyrazolone ring of PMBP is $4.01(12)^\circ$, close to the value of $3.56(3)^\circ$ found in 4-[[3,4-dihydro-5-methyl-3-oxo-2-phenyl-2*H*-pyrazol-4-ylidene(phenyl)methylamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (II) (Wang *et al.*, 2003). The bond lengths within this part of the molecule (Table 1) lie between classical single- and double-bond lengths, indicating extensive conjugation.

A strong intramolecular $N3-H3A \cdots O1$ hydrogen bond (Table 2) is observed, leading to an enamine-keto form. This case is similar to that in compound (II) [$N \cdots O = 2.745(4) \text{ \AA}$ and $N-H \cdots O = 146(4)^\circ$]. The molecule is further stabilized by intramolecular $C-H \cdots O$ and $C-H \cdots N$ hydrogen bonds (Table 2). Glide-related molecules are linked *via* $C-H \cdots O$ hydrogen-bonded chains along the *b* axis. Part of the chain structure is shown in Fig. 2.

Experimental

Compound (I) was synthesized by refluxing a mixture of 1-phenyl-3-methyl-4-benzoylpyrazol-5-one (10 mmol) and (4-fluorophenyl)methanamine (10 mmol) in ethanol (80 ml) over a steam bath for about 16 h. Excess solvent was removed by evaporation and the solution was cooled to room temperature. After 2 d, a colourless solid was obtained and this was dried in air. The product was recrystallized from ethanol to afford colourless crystals of (I) suitable for X-ray analysis.

Crystal data

$C_{24}H_{20}FN_3O$	$V = 1033.9(6) \text{ \AA}^3$
$M_r = 385.43$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.238 \text{ Mg m}^{-3}$
$a = 10.115(4) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.456(4) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 11.192(4) \text{ \AA}$	$T = 294(2) \text{ K}$
$\alpha = 98.162(6)^\circ$	Prism, colourless
$\beta = 95.571(6)^\circ$	$0.30 \times 0.24 \times 0.12 \text{ mm}$
$\gamma = 116.225(6)^\circ$	

Data collection

Bruker SMART CCD area-detector diffractometer	5308 measured reflections
φ and ω scans	3622 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1730 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.975$, $T_{\max} = 0.990$	$R_{\text{int}} = 0.038$
	$\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.057$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.168$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$
3622 reflections	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
264 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
H-atom parameters constrained	Extinction coefficient: 0.015(3)

Table 1
Selected bond lengths (\AA).

O1—C7	1.252(3)	C7—C8	1.432(4)
N3—C11	1.325(3)	C8—C11	1.398(4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N3—H3A \cdots O1	0.86	1.97	2.695 (3)	141
C1—H1 \cdots N2	0.93	2.46	2.791 (4)	101
C5—H5 \cdots O1	0.93	2.30	2.924 (4)	124
C13—H13 \cdots O1 [†]	0.93	2.60	3.430 (4)	149

Symmetry code: (i) $-x + 2, -y + 2, -z + 1$.

All H atoms were positioned geometrically, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART*; data reduction: *SAINTE* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

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

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