Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-5-(1,5-Dimethyl-3-oxo-2-phenyl-2,3-dihydro-1*H*-pyrazol-4-yliminomethyl)-2-methoxyphenyl benzenesulfonate

Xin Chen* and Ming Yu

College of Sciences, Tianjin University of Science and Technology, Tianjin 300222, People's Republic of China

Correspondence e-mail: chen_xin9999@163.com

Received 14 September 2006
Accepted 18 September 2006

In the title compound, $C_{26}H_{25}N_3O_5S$, the isovanillin group makes dihedral angles of 28.97 (6), 48.13 (7) and 70.00 (6)°, respectively, with the pyrazolone ring, the methyl-substitued benzene ring and the phenyl ring. The crystal structure contains two weak intermolecular C—H···O hydrogen bonds that link molecules into extended one-dimensional chains.

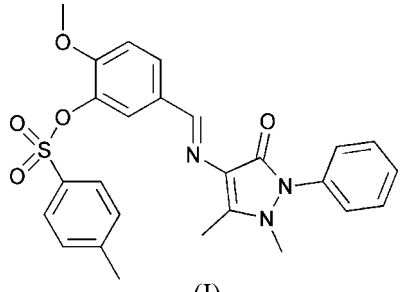
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.122
Data-to-parameter ratio = 13.4

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

Comment

Schiff-base ligands have received a good deal of attention in biology and chemistry (Kahwa *et al.*, 1986). Many Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics (Santos *et al.*, 2001). Among the large number of such compounds, 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one forms a variety of Schiff bases with aldehydes, and the syntheses and crystal structures of some of them, such as (*E*)-1,5-dimethyl-4-{2-[2-(2-nitrophenoxy)-ethoxy]benzylideneamino}-2-phenyl-1*H*-pyrazol-3(2*H*)one (Diao & Chen, 2006) and (*E*)-4-[4-(4-chlorobenzyloxy)-benzylideneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Hu, 2006), have been reported. We report here the synthesis and molecular structure of the title Schiff base compound, (I), (Fig. 1)



(I)

In the molecule of (I) (Fig. 1), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The pyrazolone ring (C16–C18/N1–N3/O5) is almost planar, with an r.m.s. deviation for the fitted atoms of 0.0329 Å. It makes a dihedral angle of 51.21 (8)° with the attached phenyl ring (C21–C26). The isovanillin group (C8–C13/C15/O3/O4) is nearly planar, with an r.m.s. deviation for the fitted atoms of 0.0368 Å. This group makes dihedral angles of 28.97 (6), 48.13 (7) and 70.00 (6)°, respectively, with the pyrazolone ring (C16–C18/N1–N3/O5), the methyl-substituted benzene ring (C1–C6) and the terminal phenyl ring (C21–C26).

The crystal packing of (I) is stabilized by weak non-classical intermolecular C—H···O hydrogen bonds (Table 1). These C—H···O hydrogen bonds link molecules into extended one-dimensional chains (Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 5-formyl-2-methoxyphenyl 4-methylbenzenesulfonate (3.06 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenylpyrazol-3-one (2.03 g, 10 mmol) and the mixture stirred at 350 K for 3 h under N_2, giving a yellow precipitate. The product was isolated, recrystallized from acetonitrile, and then dried in a vacuum to give pure compound (I) in 85% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{26}H_{25}N_3O_5S$	V = 1224.5 (4) Å^3
M_r = 491.55	Z = 2
Triclinic, $P\overline{1}$	D_x = 1.333 Mg m^{-3}
a = 9.793 (2) Å	Mo $K\alpha$ radiation
b = 9.831 (2) Å	μ = 0.17 mm^{-1}
c = 13.627 (3) Å	T = 294 (2) K
α = 79.705 (4)°	Block, yellow
β = 77.524 (4)°	0.30 × 0.24 × 0.20 mm
γ = 74.560 (3)°	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	6236 measured reflections
	4288 independent reflections
φ and ω scans	2803 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.022
	θ_{max} = 25.0°
T_{min} = 0.931, T_{max} = 0.966	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 0.1277P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.042	
$wR(F^2)$ = 0.122	
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.003
4288 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
320 parameters	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
H-atom parameters constrained	

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O5^{i}	0.93	2.43	3.229 (3)	143
C11—H11···O1^{ii}	0.93	2.56	3.475 (3)	168

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.

H atoms were included in calculated positions and refined using a riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2—H, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H.

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

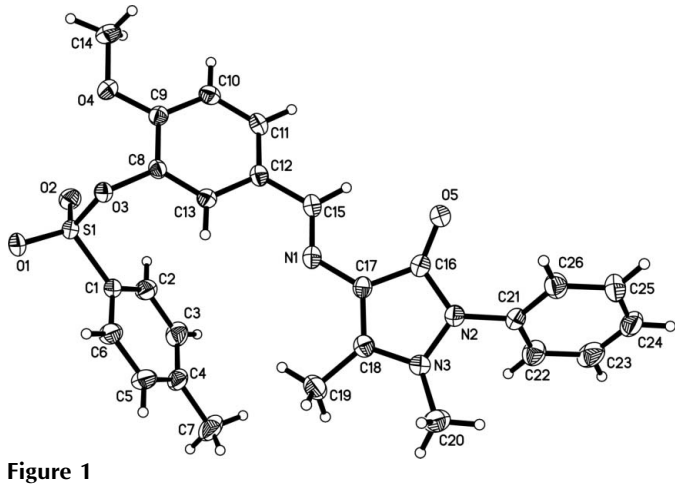


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

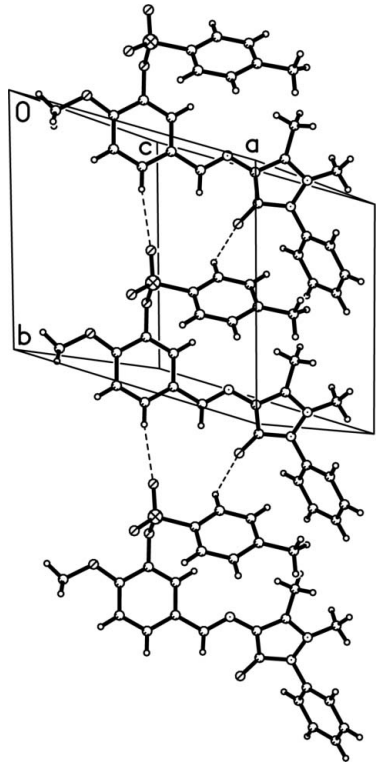


Figure 2
A packing diagram for (I), with hydrogen bonds drawn as dashed lines.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.

Diao, C.-H. & Chen, X. (2006). *Acta Cryst.* E**62**, o4422–o4424.

Hu, T.-P. (2006). *Acta Cryst.* E**62**, o2270–o2271.

Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.

Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10 for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.