Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-[(*E*)-(2,4,5-Trimethoxybenzylidene)amino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one

Hoong-Kun Fun,[a]*‡ Madhukar Hemamalini,[a] Abdullah M. Asiri[b]§ and Salman A. Khan[b]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [b]Department of Chemistry, Faculty of Science, King Abdu Aziz University, Jeddah, Saudi Arabia
Correspondence e-mail: hkfun@usm.my

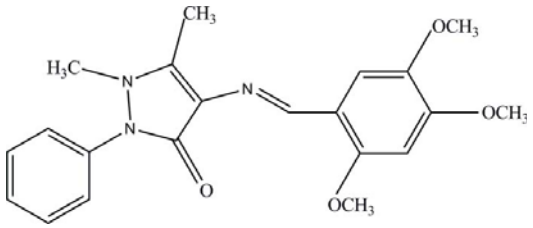
Received 1 June 2010; accepted 7 June 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.040; wR factor = 0.123; data-to-parameter ratio = 16.3.

The title compound, $C_{21}H_{23}N_3O_4$, adopts an E configuration about the central C=N double bond and the pyrazolone ring is almost planar, with a maximum deviation of 0.042 (1) Å. The central pyrazolone ring makes dihedral angles of 51.96 (5) and 3.82 (5)° with the attached phenyl and the trimethoxy-substituted benzene rings, respectively. The dihedral angle between the phenyl ring and the trimethoxy-substituted benzene ring is 50.19 (5)° and an intramolecular C—H···O hydrogen bond generates an S(6) ring motif. The crystal structure is stabilized by intermolecular C—H···O and C—H···N hydrogen bonds.

Related literature

For background to the applications of Schiff bases, see: Vukovic *et al.* (2010); Ramesh & Maheswaran (2003); Dongfang *et al.* (2008); Sastry & Rao (1988); Kamel *et al.* (2010). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{21}H_{23}N_3O_4$
M_r = 381.42
Monoclinic, $P2_1/c$
a = 21.0128 (10) Å
b = 7.4242 (4) Å
c = 12.5194 (6) Å
β = 98.675 (1)°
V = 1930.72 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.67 × 0.27 × 0.15 mm

Data collection

Bruker APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.941, T_{max} = 0.987
23600 measured reflections
5614 independent reflections
4779 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.123
S = 1.04
5614 reflections
345 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O1	0.954 (13)	2.331 (13)	3.0112 (11)	127.8 (10)
C4—H4A···O1^{i}	0.969 (13)	2.541 (13)	3.2628 (12)	131.4 (10)
C20—H20A···N3^{ii}	0.996 (14)	2.577 (14)	3.5383 (13)	162.1 (12)
C20—H20C···O2^{iii}	0.977 (14)	2.509 (14)	3.4470 (13)	160.8 (12)
C20—H20C···O3^{iii}	0.977 (14)	2.495 (15)	3.2779 (13)	137.0 (11)

Symmetry codes: (i) $x, -y-\frac{1}{2}, z+\frac{1}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and MH thank the Malaysian Government and Universiti Sains Malaysia for the Research University Golden Goose grant No. 1001/PFIZIK/811012. MH also thanks Universiti Sains Malaysia for a post-doctoral research fellowship. AMA and SAK thank the Chemistry Department, King Abdul Aziz University, Jeddah, Saudi Arabia, for providing research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5480).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Dongfang, X. U., Shuzhi, M. A., Guangying, D. U., Qizhuang, H. E. & Dazhi, S. (2008). *J. Rare Earths*, **26**, 643–647.
Kamel, M. M., Ali, H. I., Anwar, M. M., Mohamed, N. A. & Soliman, A. M. (2010). *Eur. J. Med. Chem.* **45**, 572–580.

‡ Thomson Reuters ResearcherID: A-3561-2009.
§ On secondment to: The Center of Excellence for Advanced Materials Research, King Abdu Aziz University, Jeddah 21589, Saudi Arabia.