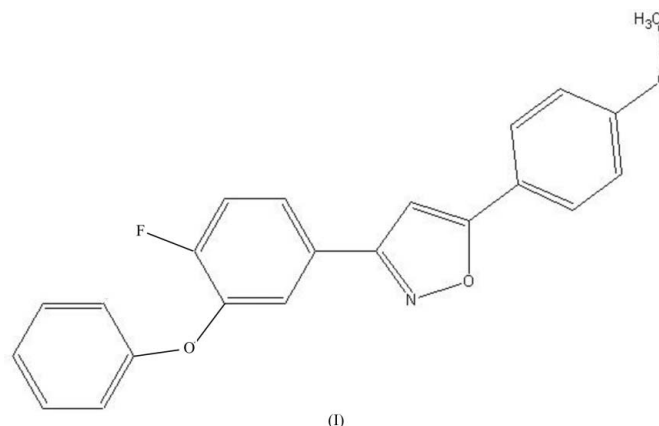


3-(4-Fluoro-3-phenoxyphenyl)-5-(4-methoxyphenyl)-
isoxazoleDeepak Chopra,^{a*} T. P. Mohan^b
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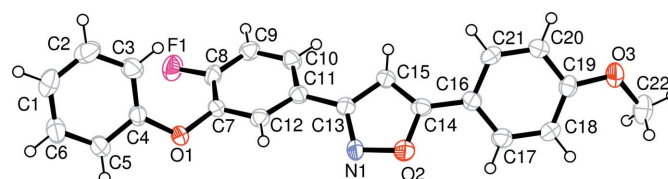
Key indicators

Single-crystal X-ray study
 $T = 290$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.067
 wR factor = 0.161
Data-to-parameter ratio = 11.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The crystal structure of the title compound, $\text{C}_{22}\text{H}_{16}\text{FNO}_3$, is
stabilized by $\text{C}-\text{H}\cdots\pi$ intermolecular interactions.Received 12 June 2006
Accepted 19 June 2006

Comment

Isoxazoles and their structure–activity relationships have been
studied for anticonvulsant activity in mice and rats (Scott *et al.*,
2006, 2006). Derivatives of isoxazoles have been also studied
as potential agrochemicals (Mohan *et al.*, 2006). We present
here the crystal structure of the title compound, (I) (Fig. 1).The bond lengths and angles (Table 1) in (I) show normal
values. The planar isoxazole makes dihedral angles of 25.0 (1)
and 27.3 (1)°, respectively, with the 4-methoxyphenyl and 4-
fluoro-3-phenoxyphenyl groups.In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\pi$ inter-
actions, involving the centroids of benzene rings C1–C6 ($Cg1$)
and C16–C21 ($Cg2$) (Table 2), pack the molecules into stacks
parallel to the b axis (Fig. 2).

Experimental

The title compound was supplied by Mohan (2006). Single crystals of
the compound were grown by slow evaporation of a dichloro-
methane–hexane (2:1 v/v) solution at 275–277 K.**Figure 1**
View of the title compound, showing the atomic numbering and 30%
probability displacement ellipsoids.

Crystal data

$C_{22}H_{16}FNO_3$
 $M_r = 361.36$
 Triclinic, $P\bar{1}$
 $a = 5.787$ (4) Å
 $b = 7.559$ (5) Å
 $c = 19.516$ (13) Å
 $\alpha = 87.527$ (12)°
 $\beta = 86.000$ (12)°
 $\gamma = 89.946$ (12)°

$V = 850.8$ (10) Å³
 $Z = 2$
 $D_x = 1.411$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 290$ (2) K
 Needle, colourless
 0.29 × 0.05 × 0.02 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.949$, $T_{max} = 0.999$

8144 measured reflections
 2971 independent reflections
 1676 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.071$
 $\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.161$
 $S = 1.03$
 2971 reflections
 249 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.101P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.20$ e Å⁻³
 $\Delta\rho_{min} = -0.20$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

F1—C8	1.355 (4)	O2—N1	1.412 (4)
O2—C14	1.352 (4)		
C17—C16—C14—C15	-152.3 (4)	N1—C13—C11—C10	-150.3 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9 \cdots Cg2 ⁱ	0.93	2.73	3.423 (5)	132
C22—H22A \cdots Cg1 ⁱⁱ	0.96	2.75	3.452 (5)	131

Symmetry codes: (i) $-x, -y + 2, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$. Cg1 and Cg2 are the centroids of benzene rings C1—C6 and C16—C21, respectively.

Atom H15 was located in a difference Fourier map and refined isotropically. All other H atoms were positioned geometrically, with C—H = 0.93–0.96 Å, and refined as riding, with $U_{iso}(H) = 1.2$ or 1.5 times $U_{eq}(C)$ for aromatic or methyl H atoms, respectively.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine

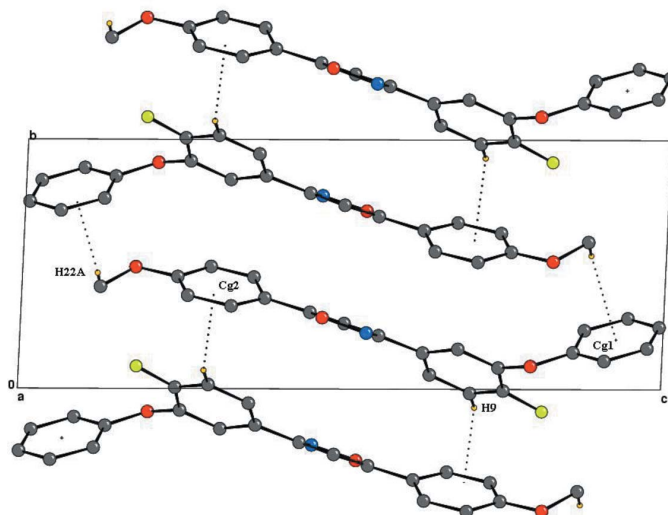


Figure 2

Packing diagram showing C—H $\cdots\pi$ interactions (dotted lines) in the bc plane. H atoms not involved in C—H $\cdots\pi$ interactions are not shown.

structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1999) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

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References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
 Bruker (2000). SMART (Version 5.628) and SAINT (Version 6.45a). Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Mohan, T. P. (2006). Thesis dissertation, Mangalore University, India.
 Scott, K. R., Butcher, R. J. & Hanson, C. D. (2006). *Acta Cryst.* **E62**, o215–o217.
 Scott, K. R., Butcher, R. J. & Hanson, C. D. (2006). *Acta Cryst.* **E62**, o218–o220.
 Sheldrick, G. M. (1996). SADABS. Version 2.03. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). SHELXL97. University of Göttingen, Germany.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
 Watkin, D. M., Pearce, L. & Prout, C. K. (1993). CAMERON. Chemical Crystallography Laboratory, University of Oxford, England.