Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(4-Methoxyphenyl)-5-(4-methylphenyl)-3-(2-pyridyl)-4*H*-1,2,4-triazole

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Received 13 March 2006
Accepted 15 March 2006

Key indicators

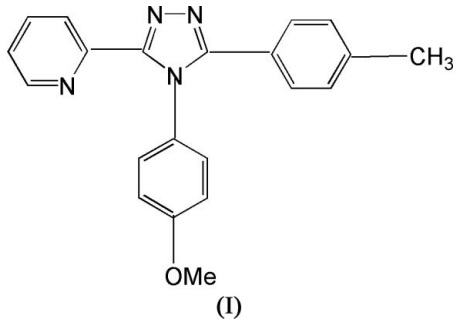
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.096
Data-to-parameter ratio = 18.3

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

In the title compound, $C_{21}H_{18}N_4O$, the *p*-methoxyphenyl and *p*-tolyl rings form dihedral angles of 61.33 (7) and 31.16 (7)°, respectively, with the triazole ring, and the dihedral angle between the triazole and pyridine rings is 46.25 (7)°. Intermolecular C—H···N hydrogen bonds link inversion-related molecules into chains.

Comment

1,2,4-Triazole and its derivatives constitute a promising class of ligands that are widely used in the synthesis of various complexes (Haasnoot, 2000). Recently, we reported the crystal structures of 1,2,4-triazole ligands and their metal complexes (Zhang *et al.*, 2004; Zhang, Liu, Ma *et al.*, 2005; Zhang, Liu, Yang *et al.*, 2005). As an extension of our work on the structural characterization of triazole derivatives, we report here the crystal structure of the title compound, (I).



(I)

In (I), the pyridine and benzene rings lie in a propeller arrangement around the central 1,2,4-triazole ring (Fig. 1), thereby minimizing the steric effects among these rings. The dihedral angles between the pyridine ring and the two benzene rings (C8–C13 and C15–C20) are 60.35 (7) and 76.37 (5)°, respectively. These two benzene rings form dihedral angles of 61.33 (7) and 31.16 (7)°, respectively, with the triazole ring, and the dihedral angle between the triazole ring and the pyridine ring is 46.25 (7)°. In the crystal structure of (I), molecules related by a center of symmetry are linked by C—H···N hydrogen bonds (Table 1 and Fig. 2), forming chains.

Experimental

Compound (I) was synthesized according to a literature method (Zhang *et al.*, 2006). Equivalent amounts of *p*-methoxyphosphazoanilide and *N*-pyridyl-*N*′-*p*-methylphenylhydrazine were reacted in ethanol (10 ml) for 1 h. After allowing the resulting solution to stand in air for 10 d, colourless crystals were formed on slow

evaporation of the solvent. The crystals were isolated, washed with ethanol and dried.

Crystal data

$C_{21}H_{18}N_4O$
M_r = 342.39
Monoclinic, $P2_1/c$
a = 11.561 (4) Å
b = 19.044 (7) Å
c = 8.540 (3) Å
β = 110.104 (6)°
V = 1765.7 (11) Å^3
Z = 4
D_x = 1.288 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2326 reflections
θ = 2.8–28.3°
μ = 0.08 mm^{-1}
T = 298 (2) K
Rod, colourless
0.24 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.981, T_{max} = 0.994
15954 measured reflections
4349 independent reflections
1628 reflections with $I > 2\sigma(I)$
R_{int} = 0.072
θ_{max} = 28.3°
$h = -15 \rightarrow 14$
$k = -25 \rightarrow 24$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.096
S = 0.92
4349 reflections
238 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0062 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···N2^{i}	0.93	2.58	3.286 (3)	133
C7—H7···N4^{ii}	0.93	2.58	3.408 (3)	148

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

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 or 0.96 Å and U_{iso}(H) = 1.2 or 1.5 (methyl) times U_{eq}(C)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

This work was supported by the Natural Science Foundation of Anhui Provincial University College (grant No. 2005KJ137).

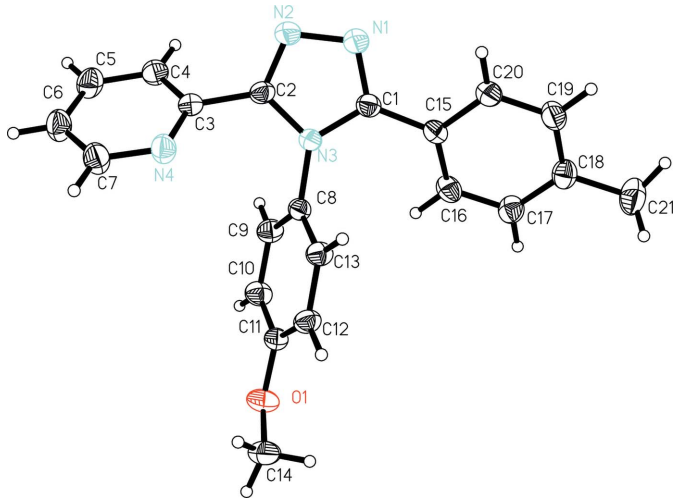


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

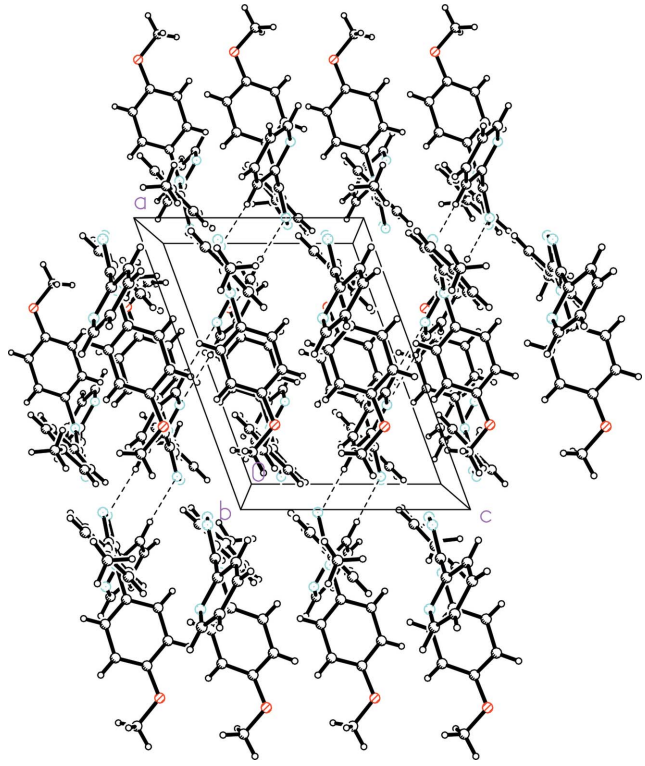


Figure 2
The crystal packing of (I), showing hydrogen-bonded (dashed lines) chains.

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