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4-(4-Ethoxyphenyl)-3,5-di-2-pyridyl-4*H*-1,2,4-triazole

Shu-Ping Zhang, Zhao-Di Liu, Song Yang, Xiao-Yang Qiu and Si-Chang Shao*

Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China

Correspondence e-mail: shaosic@fync.edu.cn

Key indicators

Single-crystal X-ray study
T = 566 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.120
Data-to-parameter ratio = 12.7

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

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In the title compound, $C_{20}H_{17}N_5O$, the two pyridyl rings form dihedral angles of 30.0 (1) and 21.0 (1)° with the triazole ring, and the dihedral angle between the triazole and benzene rings is 71.4 (1)°. The crystal packing is stabilized by C—H···N hydrogen bonds.

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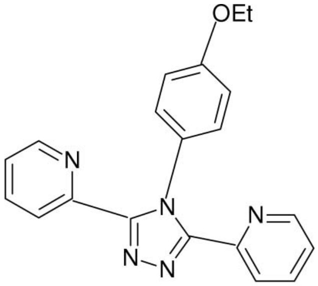
Comment

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). It is possible to produce complexes with different structures and properties, using the extensive coordinating capabilities of the N atoms of the triazole ring. We report here the crystal structure of the title compound, (I).



(I)

In (I), the pyridyl groups and the benzene ring 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 4-ethoxylphenyl ring and the two pyridyl rings (N5/C3–C7 and N4/C8–C12) are 70.9 (1) and 67.0 (1)°, respectively. The two pyridyl rings form dihedral angles of 30.0 (1) and 21.0 (1)°, respectively, with the triazole ring, and the dihedral angle between the triazole ring and the benzene ring is 71.4 (1)°. The crystal packing is stabilized by C—H···N hydrogen bonds (Table 1).

Experimental

Compound (I) was synthesized according to a literature method (Zhang *et al.*, 2004). Equivalent amounts of *p*-ethoxyphenylphosphazoanilide and *N*,*N*′-dipyridoylhydrazine were reacted in *N*,*N*′-dimethylaniline for 3 h at 463 K, with stirring. Colourless block-shaped crystals were obtained by slow evaporation of an acetone solution. The crystals were collected and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 52%). Analysis found: C 69.89, H 5.02, N 20.44%; calculated for $C_{20}H_{17}N_5O$: C 69.96, H 4.99, N 20.40%

Crystal data

$C_{20}H_{17}N_5O$
$M_r = 343.39$
Triclinic, $P\overline{1}$
$a = 8.094$ (5) Å
$b = 9.468$ (6) Å
$c = 13.152$ (8) Å
$\alpha = 104.657$ (9)°
$\beta = 92.706$ (8)°
$\gamma = 115.133$ (8)°
$V = 868.9$ (9) Å^3

$Z = 2$
$D_x = 1.312$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 1021 reflections
$\theta = 4.6$–27.3°
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
Block, white
0.20 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.983$, $T_{\max} = 0.992$
4239 measured reflections

2989 independent reflections
1790 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\max} = 25.0°$
$h = -9 \rightarrow 7$
$k = -5 \rightarrow 11$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.120$
$S = 0.87$
2989 reflections
235 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.25$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···N1$^{\rm i}$	0.93	2.46	3.308 (4)	152
C18—H18*A*···N2$^{\rm ii}$	0.93	2.53	3.459 (4)	174

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $-x+2, -y, -z$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or 1.5(methyl 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*.

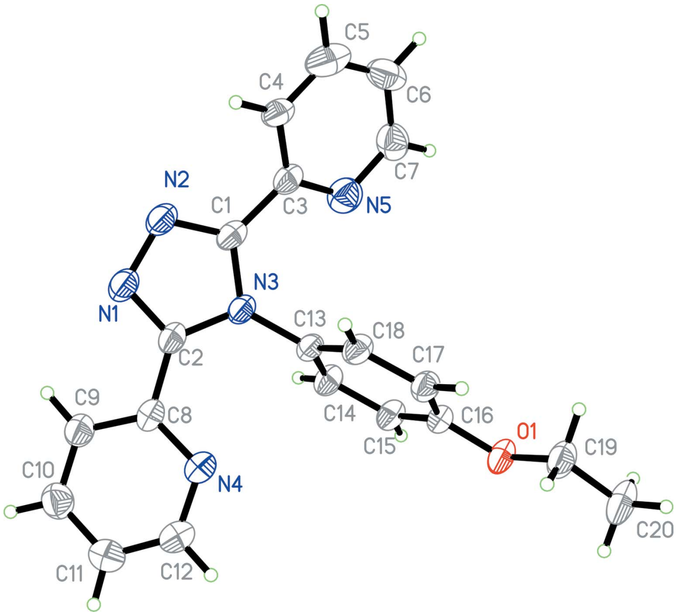


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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