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

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.049
wR factor = 0.123
Data-to-parameter ratio = 13.1

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

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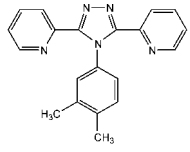
The title compound, $C_{21}H_{19}N_5$, has been synthesized and characterized by single-crystal X-ray diffraction. The dihedral angle between the benzene and triazole rings is 123.0 (5)°. The triazole ring forms dihedral angles of 36.5 (5) and 50.1 (5)° with the two pyridyl rings.

Comment

Extensive studies have been carried out on substituted 1,2,4-triazole ligands (Cornelissen *et al.*, 1992; Gupta & Bhargava, 1978; Kunkeler *et al.*, 1996). It is of interest that some iron(II) complexes containing substituted 1,2,4-triazole ligands are spin-crossover materials, which could be used as molecular-based memory devices, displays and optical switches (Garcia *et al.*, 1997; Kahn & Martinez, 1998). We have recently synthesized the title compound, (I), which can act as a potentially binucleating ligand. The present X-ray structure determination was carried out in order to elucidate the molecular conformation of (I).



(I)

Bond lengths and angles in the structure of (I) are comparable with those reported for related structures (Wang *et al.*, 1998; Chen *et al.*, 1998). The pyridyl and benzene rings lie in a propeller arrangement around the central 1,2,4-triazole ring, thereby minimizing the steric effects between these rings. The dihedral angle between the benzene and triazole rings is 123.0 (5)°. The two pyridyl rings form dihedral angles of 36.5 (5) and 50.1 (5)° with the triazole ring.

Experimental

The title compound was synthesized by the reaction of equivalent amounts of 4,4′-isopropylphenylphosphazoanilide and *N*,*N*′-dipyridylhdrazine in *N*,*N*-dimethylaniline for 3 h at 483–493 K. Single crystals suitable for X-ray diffraction analysis were obtained by evaporation of an acetone solution (Fun *et al.*, 1999).

Crystal data

$C_{20}H_{17}N_5$
M_r = 327.39
Triclinic, $P\overline{1}$
a = 10.006 (3) Å
b = 10.318 (3) Å
c = 10.371 (3) Å
α = 82.630 (5)°
β = 62.925 (5)°
γ = 63.291 (5)°
V = 847.7 (5) Å^3
Z = 2
D_x = 1.283 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 979 reflections
θ = 2.5–21.5°
μ = 0.08 mm^{-1}
T = 298 (2) K
Prism, colourless
0.32 × 0.26 × 0.20 mm

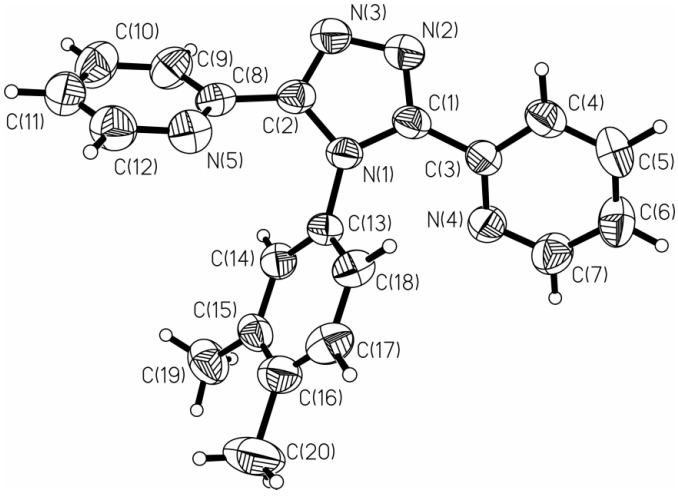


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

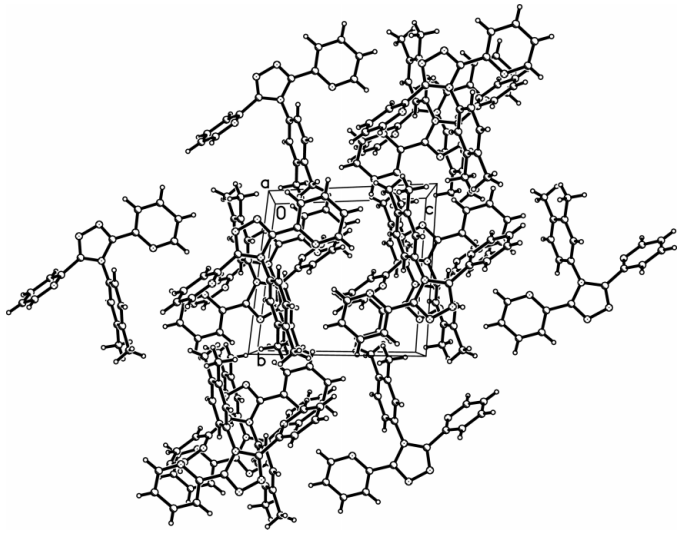


Figure 2
The molecular packing of (I), viewed along the *a* axis.

Data collection

Bruker SMART CCD area-detector diffractometer	2954 independent reflections
φ and ω scans	1530 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.023$
$T_{min} = 0.975$, $T_{max} = 0.984$	$\theta_{max} = 25.0°$
4485 measured reflections	$h = -11 \rightarrow 11$
	$k = -12 \rightarrow 5$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.123$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.26$ e Å^{-3}
2954 reflections	$\Delta\rho_{min} = -0.24$ e Å^{-3}
226 parameters	

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.365 (3)	N4—C3	1.332 (3)
N1—C1	1.369 (3)	N4—C7	1.335 (3)
N1—C13	1.442 (3)	N5—C12	1.325 (3)
N2—C1	1.317 (3)	N5—C8	1.330 (3)
N2—N3	1.380 (3)	C15—C19	1.490 (3)
N3—C2	1.314 (3)		
N2—C1—C3—N4	−143.6 (3)	C1—N1—C13—C18	58.1 (3)
N3—C2—C8—C9	49.7 (3)	C19—C15—C16—C20	−0.7 (4)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.96 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, W., Wang, Z. X., Jian, F. F., Bai, Z. P. & You, X. Z. (1998). *Acta Cryst.* C**54**, 851–852.
Cornelissen, J. P., Diemen, J. H. van, Groeneveld, L. R., Haasnoot, J. G., Spek, A. L. & Reedijk, J. (1992). *Inorg. Chem.* **31**, 198–202.
Fun, H.-K., Chinnakali, K., Shao, S. C., Zhu, D. R. & You, X. Z. (1999). *Acta Cryst.* C**55**, 770–772.
Garcia, Y., Koningsbruggen, P. J., Codjovi, E., Lapouyade, R., Kahn, O. & Rabardel, L. (1997). *J. Mater. Chem.* **7**, 857–858.
Gupta, A. K. & Bhargava, K. P. (1978). *Pharmazie*, **33**, 430–431.
Kahn, O. & Martinez, C. J. (1998). *Science*, **279**, 44–48.
Kunkeler, P. J., Koningsbruggen, P. J. van, Cornelissen, J. P., Horst, A. N. van der, Kraan, A. M. van der, Spek, A. L., Haasnoot, J. G. & Reedijk, J. (1996). *J. Am. Chem. Soc.* **118**, 2190–2197.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Wang, Z. X., Bai, Z. P., Yang, J. X., Okamoto, K. I. & You, X. Z. (1998). *Acta Cryst.* C**54**, 438–439.