

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

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Key indicators

Single-crystal X-ray study

$T = 298\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$

R factor = 0.051

wR factor = 0.147

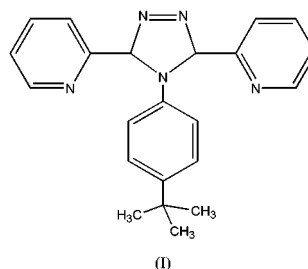
Data-to-parameter ratio = 13.5

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

The title compound, $\text{C}_{22}\text{H}_{21}\text{N}_5$, has been synthesized and characterized by single-crystal X-ray diffraction. The dihedral angle between the benzene and triazole rings of the title compound is $117.6(5)^\circ$. The triazole ring forms dihedral angles of $25.2(5)$ and $136.7(5)^\circ$ 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 molecule, (I), which can act as a potentially dinucleating ligand. The present X-ray structure determination was carried out in order to elucidate the molecular conformation.



Bond lengths and angles in the structure are comparable with those reported for related structures (Wang *et al.*, 1998; Chen *et al.*, 1998; Fun *et al.*, 1999). The pyridyl groups and the

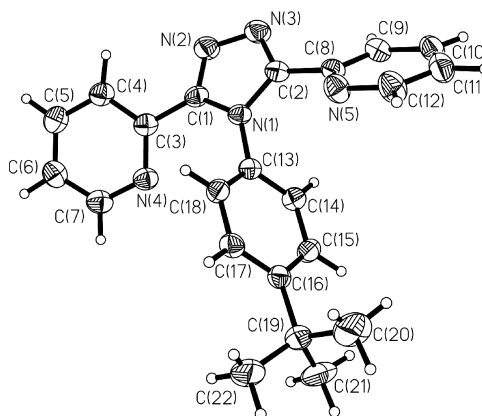


Figure 1

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

benzene ring lie in a propeller arrangement around the central 1,2,4-triazole ring, thereby minimizing the steric effects among these rings. The dihedral angle between the planes of the benzene and triazole rings is $117.6(5)^\circ$. The two pyridyl rings form dihedral angles of $25.2(5)$ and $136.7(5)^\circ$ with the triazole ring.

Experimental

The title compound was synthesized by the reaction of equivalent amounts of 4,4'-*p*-(*tert*-butyl)phenylphosphazooanilide and *N,N'*-dipyridoylhydrazine 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.

Crystal data

$C_{22}H_{21}N_5$	$D_x = 1.260 \text{ Mg m}^{-3}$
$M_r = 355.44$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 1760 reflections
$a = 15.348(9) \text{ \AA}$	$\theta = 3.0\text{--}20.9^\circ$
$b = 5.980(3) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 20.909(12) \text{ \AA}$	$T = 298(2) \text{ K}$
$\beta = 102.488(9)^\circ$	Prism, colorless
$V = 1873.7(18) \text{ \AA}^3$	$0.45 \times 0.33 \times 0.29 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	3291 independent reflections
φ and ω scans	1729 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.042$
$T_{\text{min}} = 0.966$, $T_{\text{max}} = 0.978$	$\theta_{\text{max}} = 25.0^\circ$
9340 measured reflections	$h = -18 \rightarrow 18$
	$k = -7 \rightarrow 6$
	$l = -21 \rightarrow 24$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.051$	$w = 1/[\sigma^2(F_o^2) + (0.0721P)^2]$
$wR(F^2) = 0.147$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.96$	$(\Delta/\sigma)_{\text{max}} < 0.001$
3291 reflections	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
244 parameters	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

N1—C1	1.372(3)	N4—C7	1.337(3)
N1—C2	1.373(3)	N4—C3	1.339(3)
N1—C13	1.437(3)	N5—C8	1.335(3)
N2—C1	1.304(3)	N5—C12	1.335(4)
N2—N3	1.386(3)	C16—C19	1.517(4)
N3—C2	1.304(3)		
N2—C1—C3—N4	155.9(3)	C1—N1—C13—C18	-68.8(3)
N3—C2—C8—C9	-44.0(4)		

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998) and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick,

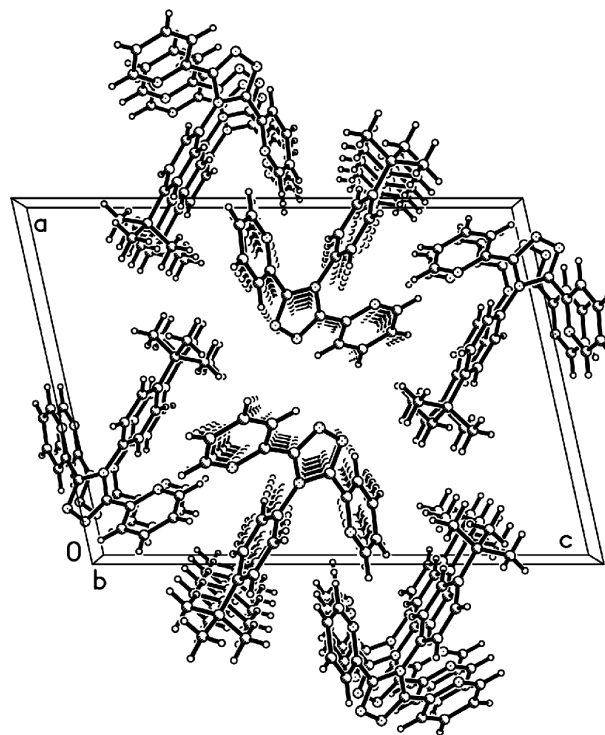


Figure 2

The molecular packing of (I), viewed along the *b* axis.

1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, China, for research grant No. 2003 kJ681.

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. C54*, 851–852.
- Cornelissen, J. P., van Diemen, J. H., 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. C55*, 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., van Koningsbruggen, P. J., Cornelissen, J. P., vander Horst, A. N., vander Kraan, A. M., 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). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Wang, Z. X., Bai, Z. P., Yang, J. X., Okamoto, K. I. & You, X. Z. (1998). *Acta Cryst. C54*, 438–439.