

4-Phenyl-3,5-bis(2-pyridyl)-4*H*-1,2,4-triazole

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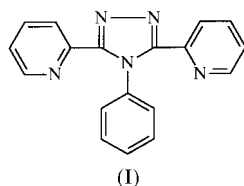
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In the title compound, $C_{18}H_{13}N_5$, the two pyridyl rings form dihedral angles of 32.7 (2) and 30.1 (2)° with the triazole ring. The most favoured orientation of the pyridyl rings is that with their N atoms on opposite sides of the triazole ring directed towards the phenyl ring. π - π -Stacking interactions involving pyridyl rings are observed along the *a* axis at a perpendicular distance of 3.670 (3) Å. This arrangement is further stabilized by weak intermolecular C—H...N hydrogen bonds.

Comment

Substituted 1,2,4-triazoles have been actively studied as bridging ligands coordinating through their vicinal N atoms. It is of interest that some complexes containing 1,2,4-triazole ligands have particular structures and specific magnetic properties (Vreugdenhil *et al.*, 1987; Albada *et al.*, 1984; Vos *et al.*, 1983; Kahn & Martinez, 1998). On the other hand, some of the 1,2,4-triazole derivatives have anti-inflammatory activities (Mazzone *et al.*, 1987) and some are antifungal agents (Massa *et al.*, 1992). As a continuation of our investigation of the structures of triaryltriazole compounds (Wang *et al.*, 1998; Chen *et al.*, 1998; Fun *et al.*, 1999; Shao *et al.*, 1999), we describe herein the structure of the title compound, (I).



The title structure (Fig. 1) consists of two pyridyl rings, one triazole ring and one phenyl ring. The four rings do not share a common plane; the dihedral angle between the phenyl and central triazole rings is 65.2 (3)°, and the pyridyl rings form dihedral angles of 32.7 (2) and 30.1 (2)° with the triazole ring. The most favoured orientation of the pyridyl rings is that with their N atoms on opposite sides of the triazole-ring plane and oriented towards the phenyl ring. This orientation is due to the weak hydrogen-bond interactions in which the pyridyl and

triazole rings are involved, in particular the C4—H4...N3 and C9—H9...N4 interactions (Table 2). Bond lengths and angles in (I) are comparable with those reported for related structures (Wang *et al.*, 1998; Fun *et al.*, 1999). In contrast to these related structures, however, in (I), intermolecular π - π stacking interactions between the N1-pyridyl ring and its symmetry partner at (1 - *x*, 2 - *y*, 1 - *z*) are observed along the *a* axis, with a perpendicular distance of 3.670 (3) Å. This arrangement is further stabilized by weak intermolecular C17—H17...N4 and C11—H11...N3 hydrogen bonds. The geometry of these interactions is given in Table 2.

In order to investigate how far packing interactions can influence the conformation of the molecule, molecular-mechanics calculations were carried out using the MM^+ force field of *HYPERCHEM* (Autodesk Inc., 1992). The best calculated model for the isolated molecule so obtained differs from that found experimentally for the molecule packed in the crystal because in the isolated molecule, the two pyridyl rings are practically coplanar with the central triazole ring, while in the crystal, they are rotated by an angle of about 32°. Another relevant difference is shown by the plane of the phenyl ring which is practically perpendicular to the plane of the triazole ring in the isolated molecule, while it is twisted by about 65° in the crystal. This means that conjugation between the two pyridyl and triazole rings is favoured in the isolated molecule, but is in some way hindered by interactions with the surrounding molecules in the crystal. Conjugation with the phenyl ring is hindered in both cases.

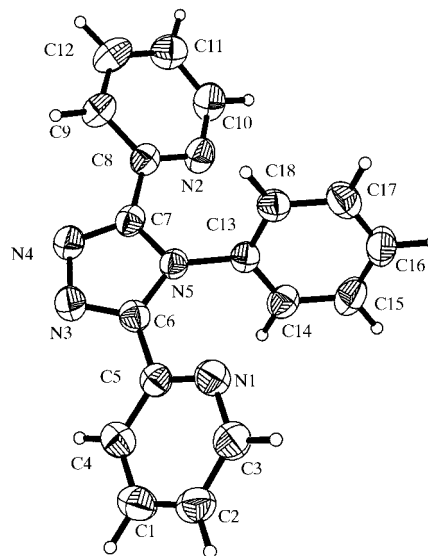


Figure 1

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

Experimental

The title compound was prepared by the reaction of equivalent amounts of 4,4'-phenylphosphazoanilide and *N,N'*-dipyridylhydrazine in *N,N'*-dimethylaniline for 3 h at 463–473 K (Grimmel *et al.*, 1946; Klingsberg, 1958). Diffraction-quality crystals were obtained by recrystallization from acetone.

Crystal data

$C_{18}H_{13}N_5$	$D_x = 1.376 \text{ Mg m}^{-3}$
$M_r = 299.33$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 57 reflections
$a = 5.9217 (8) \text{ \AA}$	$\theta = 6.73\text{--}12.50^\circ$
$b = 15.3265 (15) \text{ \AA}$	$\mu = 0.087 \text{ mm}^{-1}$
$c = 15.9824 (14) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 95.188 (10)^\circ$	Block, colourless
$V = 1444.6 (3) \text{ \AA}^3$	$0.58 \times 0.25 \times 0.22 \text{ mm}$
$Z = 4$	

Data collection

Siemens P4 diffractometer	$h = -1 \rightarrow 7$
$2\theta/\omega$ scans	$k = -1 \rightarrow 18$
3576 measured reflections	$l = -18 \rightarrow 18$
2531 independent reflections	3 standard reflections
1800 reflections with $I > 2\sigma(I)$	every 97 reflections
$R_{\text{int}} = 0.028$	intensity decay: 6.81%
$\theta_{\text{max}} = 25^\circ$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 0.1874P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.109$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.006$	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
2531 reflections	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$
261 parameters	Extinction correction: <i>SHELXL97</i>
All H-atom parameters refined	Extinction coefficient: 0.0124 (18)

Table 1

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

N1—C3	1.343 (3)	N3—N4	1.378 (2)
N1—C5	1.345 (2)	N4—C7	1.316 (2)
N2—C10	1.339 (3)	N5—C7	1.372 (2)
N2—C8	1.343 (3)	N5—C6	1.372 (2)
N3—C6	1.316 (2)	N5—C13	1.449 (2)
C6—N3—N4	107.5 (2)	N3—C6—C5	122.0 (2)
C7—N4—N3	107.4 (2)	N5—C6—C5	127.8 (2)
C7—N5—C6	104.5 (2)	N4—C7—N5	110.3 (2)
N3—C6—N5	110.3 (2)	N4—C7—C8	121.8 (2)

Table 2

Hydrogen-bonding and short contact geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C4—H4 \cdots N3	0.95 (2)	2.65 (2)	2.904 (3)	96 (2)
C9—H9 \cdots N4	1.00 (2)	2.61 (2)	2.886 (3)	96 (1)
C17—H17 \cdots N4 ⁱ	0.96 (2)	2.67 (2)	3.490 (3)	143 (2)
C11—H11 \cdots N3 ⁱⁱ	0.98 (3)	2.64 (3)	3.437 (3)	138 (2)

Symmetry codes: (i) $x - \frac{1}{2}, \frac{3}{2} - y, z - \frac{1}{2}$; (ii) $-\frac{1}{2} - x, y - \frac{1}{2}, \frac{3}{2} - z$.

The H atoms were located from the different Fourier map and were refined isotropically; C—H distances are in the range 0.95 (2)–1.02 (3) \AA .

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1465). Services for accessing these data are described at the back of the journal.

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