

## 5,7-Diphenyltetrazolo[1,5-a]pyridine-8-carbonitrile

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In the title molecule, C<sub>18</sub>H<sub>11</sub>N<sub>5</sub>, the planar tetrazole ring is nearly coplanar with the pyridine-ring plane. The crystal structure is stabilized by  $\pi \cdots \pi$  and C—H $\cdots\pi$  interactions

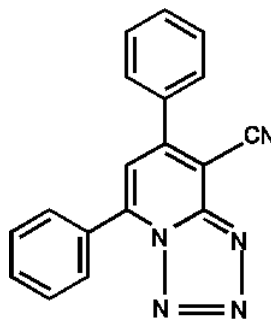
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### Comment

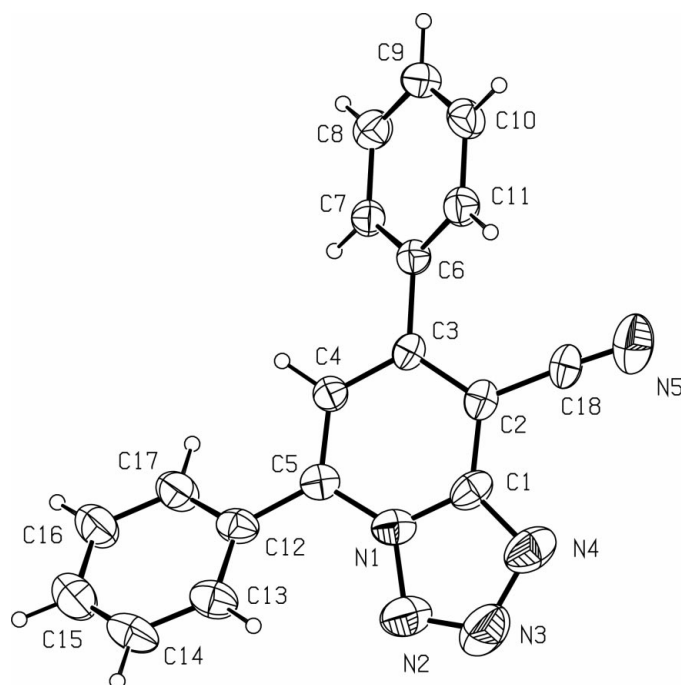
Tetrazolopyridines are fused heterocyclic compounds in which the tetrazole ring is fused to a  $\pi$ -deficient pyridine nucleus. This class of compounds are very important as reduction leads to the formation of various aminopyridines (Mekheimer, 1994); the latter constitute a class of nitrogen heterocycles used in the agrochemical and pharmaceutical industries (Vijn *et al.*, 1993). Here we report the crystal structure of a novel tetrazolopyridine, (I).



(I)

The bond lengths and angles observed in (I) (Fig. 1) are normal. The tetrazole ring is planar within  $\pm 0.011$  (4) Å. The pyridine and the two phenyl rings are each planar, with atoms C2, C6 and C12 deviating most, by 0.012 (3), 0.013 (3) and 0.017 (3) Å, respectively. The pyridine and tetrazole rings are nearly coplanar, with a dihedral angle of 1.9 (2)°. The phenyl rings C6–C11 and C12–C17 form dihedral angles of 42.4 (2) and 32.6 (2)°, respectively, with the pyridine ring. The geometry of the tetrazole ring is in good agreement with that observed in similar compounds having a fused tetrazole ring (Golič *et al.*, 1978, 1994; Katrusiak *et al.*, 1997).

In the crystal, the molecular packing is stabilized by  $\pi \cdots \pi$ -stacking interactions and C—H $\cdots\pi$  interactions. The pyridine ring and a phenyl ring of the symmetry-related molecule at  $(1-x, 1/2+y, 3/2-z)$  are stacked with their centroids separated by a distance of 3.592 (2) Å. A C—H $\cdots\pi$  interaction involving C14 and one of the phenyl rings is observed, such that H14 $\cdots$ Cg = 2.92 Å, C14 $\cdots$ Cg = 3.594 (5) and C14—H14 $\cdots$ Cg = 130°, where Cg is the centre of gravity of phenyl ring C12–C17 at  $(2-x, -1/2+y, 3/2-z)$ .



**Figure 1**  
The structure of (I), showing 30% probability displacement ellipsoids.

## Experimental

The title compound, (I), was synthesized, according to the method of Shah (2000), from 4,6-diphenyl-2-chloronicotinonitrile, using sodium azide as a nucleophilic agent. The reaction was performed under liquid–liquid phase-transfer conditions, using chlorobenzene as a solvent and tricaprylmethylammonium chloride as a phase-transfer catalyst. Thin needle-shaped crystals of the compound were grown from a hot methanol solution by slow evaporation.

### Crystal data

$C_{18}H_{11}N_5$   
 $M_r = 297.32$   
 Monoclinic,  $P2_1/c$   
 $a = 13.3861$  (10) Å  
 $b = 7.522$  (2) Å  
 $c = 15.109$  (3) Å  
 $\beta = 102.12$  (2)°  
 $V = 1487.4$  (5) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.328$  Mg m<sup>-3</sup>  
 $D_m = 1.311$  (5) Mg m<sup>-3</sup>

### Data collection

Enraf–Nonius CAD-4  
 diffractometer  
 $\omega$ -2 $\theta$  scans  
 Absorption correction:  $\psi$  scan  
 (North *et al.*, 1968)  
 $T_{\min} = 0.990$ ,  $T_{\max} = 0.992$   
 2839 measured reflections  
 2600 independent reflections  
 1347 reflections with  $I > 2\sigma(I)$

$D_m$  measured by flotation in an  
 aqueous potassium iodide  
 solution  
 Mo  $K\alpha$  radiation  
 Cell parameters from 25  
 reflections  
 $\theta = 25$ – $35^\circ$   
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Needle, colourless  
 $0.2 \times 0.1 \times 0.1$  mm

$R_{\text{int}} = 0.041$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = -15 \rightarrow 15$   
 $k = 0 \rightarrow 8$   
 $l = -17 \rightarrow 17$   
 2 standard reflections  
 frequency: 60 min  
 intensity decay: 1%

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.185$   
 $S = 0.96$   
 2600 reflections  
 208 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0936P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.46$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.18$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å).

|       |           |        |           |
|-------|-----------|--------|-----------|
| N1–C1 | 1.346 (4) | N3–N4  | 1.435 (5) |
| N1–C5 | 1.377 (4) | N4–C1  | 1.324 (4) |
| N1–N2 | 1.404 (4) | N5–C18 | 1.107 (4) |
| N2–N3 | 1.267 (4) |        |           |

The highest difference peak is much larger than the absolute value of the deepest hole. The difference Fourier map showed that the highest three peaks were close to the N atoms. The positions of these peaks and the large displacement parameters for all the N atoms suggested a rotational disorder for the tetrazole ring and the carbonitrile group about the C1–N4 bond. Attempts to refine the structure by using a disorder model did not give satisfactory results. Hence the present model was retained.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *MolEN* (Fair, 1990); data reduction: *MolEN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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