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5,6-Diphenyl-3-(2-pyridyl)-1,2,4-triazine

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In the title compound, $C_{20}H_{14}N_4$, the triazine ring adopts a slight twist conformation. In the crystal structure, intermolecular C—H···N interactions connect the molecules into chains along the *b* axis. The crystal packing is also stabilized by π–π and C—H···π interactions.

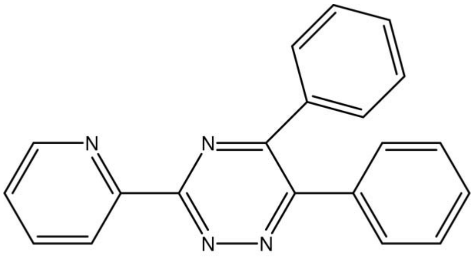
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.047
wR factor = 0.131
Data-to-parameter ratio = 24.8

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

Comment

3,5,6-Trisubstituted-1,2,4-triazines, such as the title compound, (I), represent a principal class of *N*-donor heterocyclic ligands that exhibit interesting pharmacological properties such as blood platelet aggregation inhibition, antiviral, anti-HIV and anticancer (leukemia and ovarian) activity (Soudi *et al.*, 2005; Mashaly *et al.*, 1999). 1,2,4-Triazines have also been used in analytical chemistry to determine the concentration of some trace metal ions (Almog *et al.*, 1996; Croot & Hunter, 2000).


(I)

Bond lengths and angles in (I) (Fig. 1) have normal values (Allen *et al.*, 1987). The C15–C20 and C9–C14 phenyl rings are attached to the triazine ring at atoms C3 and C2, with torsion angles N3—C3—C15—C20 = 51.09 (12)° and C3—C2—C9—C14 = 33.36 (14)°. The triazine ring adopts a slight twist conformation, with puckering parameters (Cremer & Pople, 1975) Q = 0.097 (1) Å, θ = 92.2 (6) and φ_2 = 333.1 (5)°.

In the crystal structure, the molecules are linked by intermolecular C—H···N intermolecular interactions, forming chains along the *b* axis (Table 1 and Fig. 2). The crystal packing is stabilized by C—H···π interactions (Table 1) involving the triazine ring (centroid *Cg* 1) and the C4/N4/C5–C8 (centroid *Cg*2), C9–C14 (centroid *Cg*3) and C15–C20 (centroid *Cg*4) phenyl rings. In addition, the crystal structure is further stabilized by π–π interactions involving the triazine ring at (x, y, z) and C4/N4/C5–C8 at ($-x$, $2 - y$, $-z$), with a centroid–centroid distance of 3.5434 (6) Å.

Experimental

Recently, we reported the crystal structure of the Mn^{II} and Cd^{II} complexes of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine (Eltayeb, Teoh

& Yamin, 2006; Eltayeb, Teoh, Teh *et al.*, 2006) and planned to prepare the Zn^{II} complex by stirring 5,6-diphenyl-3-(2-pridyl)-1,2,4-triazine (0.310 g, 1.0 mmol), as purchased from Acros, and $ZnCl_2$ (0.68 g, 0.5 mmol) together at room temperature for 1 h in a mixture of 20 ml of CH_2Cl_2 and 10 ml of THF. The resulting yellow solution was filtered, and yellow crystals formed after a few days of slow evaporation of the solvent at room temperature. Unfortunately, the crystals were of the starting materal and not the Zn^{II} complex.

Crystal data

$C_{20}H_{14}N_4$
$M_r = 310.35$
Monoclinic, $P2_1/c$
$a = 11.5830$ (3) Å
$b = 11.0381$ (2) Å
$c = 11.9550$ (3) Å
$\beta = 94.127$ (1)°
$V = 1524.53$ (6) Å^3
$Z = 4$
$D_x = 1.352$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 100.0$ (1) K
Block, yellow
0.64 × 0.21 × 0.20 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.887$, $T_{max} = 0.984$
38592 measured reflections
5386 independent reflections
4472 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 32.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.131$
$S = 1.03$
5386 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0737P)^2 + 0.4168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···N4^{i}	0.93	2.52	3.322 (1)	145
C6—H6A···Cg4^{i}	0.93	2.82	3.470 (1)	128
C13—H13A···Cg1^{ii}	0.93	3.00	3.487 (1)	115
C14—H14A···Cg1^{ii}	0.93	3.32	3.661 (1)	104
C17—H17A···Cg3^{iii}	0.93	2.65	3.478 (1)	149
C20—H20A···Cg2^{ii}	0.93	3.10	3.685 (1)	122

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y+1, -z$. Cg1, Cg2, Cg3 and Cg4 are the centroids of the triazine, C4/N4/C5–C8, C9–C14 and C15–C20 rings, respectively.

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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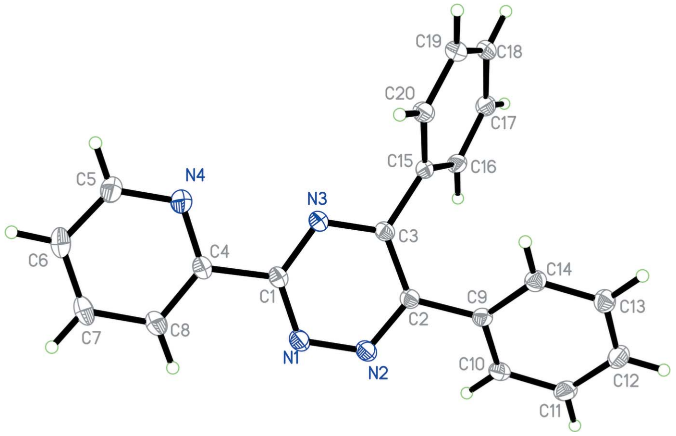

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

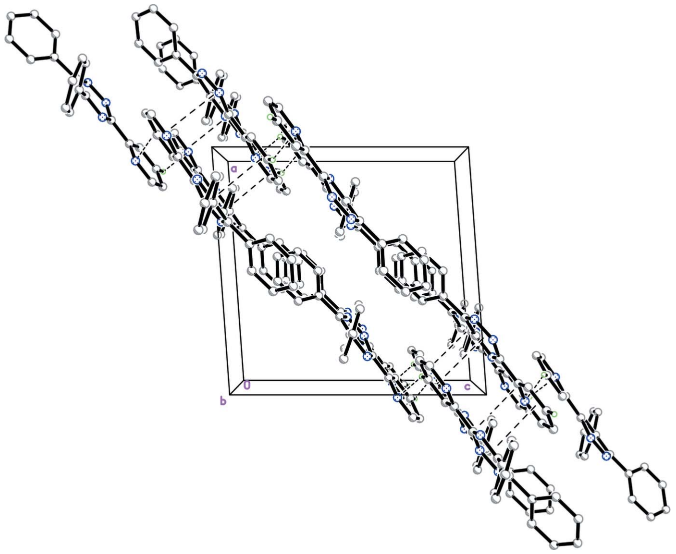

Figure 2
The crystal packing of (I), with intermolecular C—H··· N hydrogen bonds and π–π interactions shown as dashed lines.

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