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

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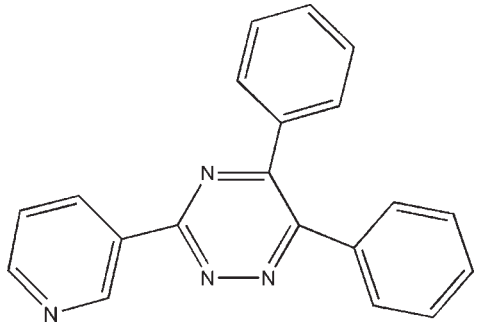
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.125; data-to-parameter ratio = 17.3.

In the molecule of the title compound, $C_{20}H_{14}N_4$, the triazine ring is attached to two phenyl rings and one pyridine ring. In the crystal, molecules are linked by intermolecular C—H···N hydrogen bonds. The crystal packing is also stabilized by C—H···π interactions.

Related literature

For applications of substituted 1,2,4-triazines, see: Denecke *et al.* (2005); Maheshwari *et al.* (2006): Zhao *et al.* (2003).



Experimental

Crystal data

$C_{20}H_{14}N_4$
M_r = 310.35
Monoclinic, $P2_1/c$
a = 14.4775 (16) Å
b = 7.0923 (8) Å
c = 18.5786 (15) Å
β = 125.587 (6)°
V = 1551.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.31 × 0.28 × 0.26 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
9802 measured reflections
3770 independent reflections
2184 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
3 standard reflections every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.125
S = 1.04
3770 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the N4,C16–C20 and C1–C6 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20A···N3	0.93	2.49	2.824 (4)	102
C13—H13A···$Cg1^{i}$	0.93	3.49	3.345 (4)	91
C19—H19A···$Cg2^{ii}$	0.93	3.67	3.109 (4)	121

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL/PC* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2609).

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supporting information

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

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S1. Comment

The increasing interest in the chemistry of substituted 1,2,4-triazine is due to their various applications: commercial dyes, herbicides (Zhao *et al.*, 2003), antiviral, antitumor drug (Maheshwari *et al.*, 2006) and selective extracting agents in the separation of lanthanides and actinides in the management of nuclear wastes (Denecke *et al.*, 2005). The title compound belongs to the family of these compounds. We have synthesized the title compound and describe its structure here.

In the title compound, the bond lengths and angles are generally normal. The dihedral angles between triazine ring(p1) with the pyridine ring (p2), C1—C6 (p3) and C9—C14 (p4) phenyl rings are 2.94 (2)°, 53.35 (2)° and 50.43 (2)°, respectively. There exist intermolecular C—H···N hydrogen bond and C—H···π supramolecular interactions in the crystal lattice. The donor and acceptor distance is 2.8235Å for C20—H20A···N3. In addition, there are obvious intermolecular C—H···π interactions between C13—H13A and pyridine ring (*Cg*(2)), C19—H19A and C1—C6 phenyl ring (*Cg*(3)). In the solid state, all above intermolecular interactions in the title compound stabilize the crystal packing structure.

S2. Experimental

To a mixture of (3-pyridylcarbonyl)hydrazine (0.828 g, 6 mmol) and benzil (1.26 g, 6 mmol) was added ammonium acetate (4.62 g, 0.06 mol) and 1 ml of acetic acid. The mixture was heated by conventional microwave oven for 5 min at 453 K. Upon rapid cooling of the reaction vessel to 313 K, a yellow precipitate formed, which was washed with water to afford the title compound (yield 45.3%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature for three days.

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of 0.93–0.96 Å, respectively, and with U_{iso}(H) = 1.2U_{eq} of the parent atoms.

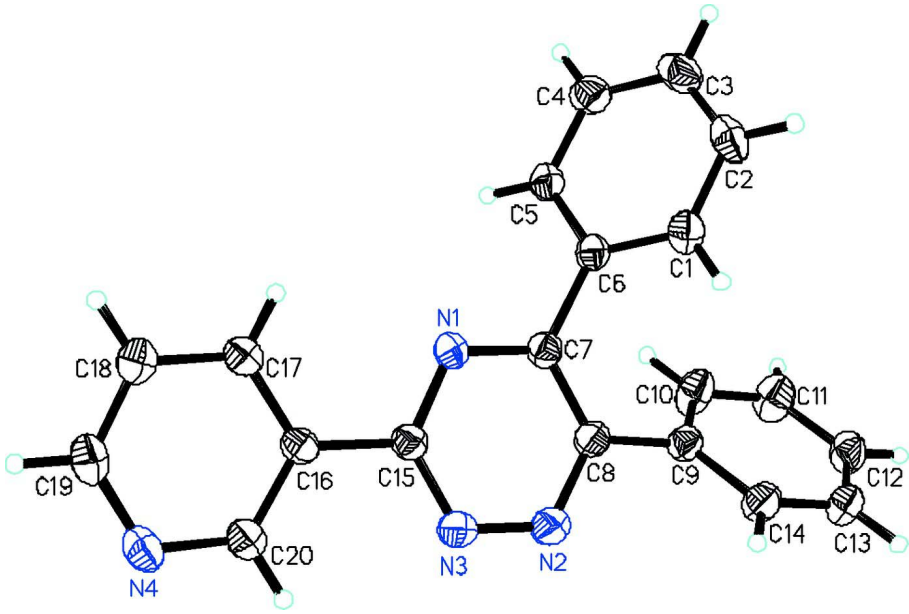

Figure 1

The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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

Crystal data

$C_{20}H_{14}N_4$
$M_r = 310.35$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.4775\ (16)$ Å
$b = 7.0923\ (8)$ Å
$c = 18.5786\ (15)$ Å
$\beta = 125.587\ (6)°$
$V = 1551.3\ (3)$ Å^3
$Z = 4$

$F(000) = 648$
$D_x = 1.329$ Mg m^{-3}
Melting point: 444 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 1.7–28.3°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Block, yellow
0.31 × 0.28 × 0.26 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
9802 measured reflections
3770 independent reflections
2184 reflections with $I > 2\sigma(I)$

$R_{int} = 0.033$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.7°$
$h = -16\rightarrow19$
$k = -7\rightarrow9$
$l = -24\rightarrow20$
3 standard reflections every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.125$

$S = 1.04$
3770 reflections
218 parameters
0 restraints

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0105 (17)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.40833 (10)	0.74465 (17)	0.84881 (7)	0.0422 (3)
N2	0.48148 (11)	0.5785 (2)	0.75648 (8)	0.0554 (4)
N3	0.55312 (11)	0.5984 (2)	0.84483 (8)	0.0546 (4)
C20	0.69841 (13)	0.6021 (2)	1.03161 (9)	0.0505 (4)
H20A	0.7215	0.5456	0.9993	0.061*
C1	0.19450 (14)	0.9625 (2)	0.65096 (9)	0.0512 (4)
H1B	0.2415	0.9897	0.6334	0.061*
C2	0.09076 (15)	1.0535 (2)	0.61123 (10)	0.0598 (5)
H2B	0.0688	1.1431	0.5674	0.072*
C3	0.02025 (14)	1.0123 (3)	0.63613 (10)	0.0608 (5)
H3B	−0.0496	1.0727	0.6087	0.073*
C4	0.05291 (13)	0.8823 (2)	0.70138 (10)	0.0555 (4)
H4B	0.0050	0.8541	0.7180	0.067*
C5	0.15676 (12)	0.7931 (2)	0.74260 (9)	0.0475 (4)
H5A	0.1793	0.7073	0.7879	0.057*
C6	0.22752 (12)	0.8308 (2)	0.71683 (9)	0.0410 (4)
C7	0.33957 (11)	0.7350 (2)	0.76126 (8)	0.0398 (4)
C8	0.37453 (12)	0.6390 (2)	0.71427 (9)	0.0430 (4)
C9	0.29850 (13)	0.5980 (2)	0.61817 (9)	0.0437 (4)
C10	0.19430 (15)	0.5132 (3)	0.58174 (10)	0.0625 (5)
H10A	0.1710	0.4833	0.6176	0.075*
C11	0.12424 (16)	0.4725 (3)	0.49224 (11)	0.0692 (5)
H11A	0.0546	0.4141	0.4684	0.083*
C12	0.15742 (15)	0.5181 (2)	0.43853 (10)	0.0581 (5)
H12A	0.1102	0.4912	0.3783	0.070*
C13	0.25980 (15)	0.6030 (2)	0.47375 (10)	0.0578 (5)
H13A	0.2819	0.6354	0.4373	0.069*
C14	0.33114 (14)	0.6412 (2)	0.56364 (10)	0.0531 (4)

H14A	0.4016	0.6964	0.5874	0.064*
C15	0.51278 (12)	0.6718 (2)	0.88740 (9)	0.0410 (4)
C16	0.59002 (12)	0.6778 (2)	0.98515 (9)	0.0400 (4)
C17	0.55691 (13)	0.7604 (2)	1.03439 (9)	0.0506 (4)
H17A	0.4845	0.8112	1.0062	0.061*
C18	0.63165 (14)	0.7668 (2)	1.12525 (10)	0.0569 (5)
H18A	0.6111	0.8231	1.1592	0.068*
C19	0.73715 (14)	0.6882 (2)	1.16431 (10)	0.0575 (5)
H19A	0.7876	0.6932	1.2257	0.069*
N4	0.77171 (11)	0.6048 (2)	1.11941 (8)	0.0585 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0368 (7)	0.0495 (8)	0.0368 (6)	0.0013 (6)	0.0193 (5)	−0.0009 (6)
N2	0.0498 (9)	0.0713 (10)	0.0462 (8)	0.0062 (7)	0.0285 (7)	−0.0046 (7)
N3	0.0434 (8)	0.0729 (10)	0.0452 (8)	0.0091 (7)	0.0244 (7)	−0.0038 (7)
C20	0.0439 (9)	0.0556 (10)	0.0456 (9)	0.0041 (7)	0.0223 (8)	0.0010 (8)
C1	0.0526 (10)	0.0574 (10)	0.0405 (8)	−0.0012 (8)	0.0254 (7)	0.0024 (8)
C2	0.0567 (11)	0.0541 (11)	0.0424 (9)	0.0059 (8)	0.0138 (8)	0.0065 (8)
C3	0.0386 (9)	0.0666 (12)	0.0519 (10)	0.0081 (8)	0.0119 (8)	−0.0059 (9)
C4	0.0402 (9)	0.0705 (12)	0.0524 (10)	−0.0002 (8)	0.0249 (8)	−0.0068 (9)
C5	0.0436 (9)	0.0577 (10)	0.0378 (8)	0.0035 (7)	0.0217 (7)	0.0029 (7)
C6	0.0372 (8)	0.0486 (9)	0.0319 (7)	−0.0006 (7)	0.0171 (6)	−0.0040 (6)
C7	0.0375 (8)	0.0436 (9)	0.0371 (8)	−0.0029 (6)	0.0210 (7)	−0.0006 (6)
C8	0.0421 (8)	0.0484 (9)	0.0400 (8)	−0.0013 (7)	0.0248 (7)	−0.0011 (7)
C9	0.0477 (9)	0.0442 (9)	0.0414 (8)	0.0003 (7)	0.0271 (7)	−0.0027 (7)
C10	0.0674 (12)	0.0758 (13)	0.0490 (10)	−0.0227 (10)	0.0366 (9)	−0.0126 (9)
C11	0.0671 (12)	0.0810 (14)	0.0546 (11)	−0.0240 (10)	0.0326 (10)	−0.0166 (9)
C12	0.0664 (12)	0.0608 (11)	0.0397 (9)	0.0004 (9)	0.0267 (8)	−0.0065 (8)
C13	0.0681 (12)	0.0670 (12)	0.0479 (10)	0.0031 (9)	0.0392 (9)	0.0005 (8)
C14	0.0526 (10)	0.0626 (11)	0.0492 (9)	−0.0026 (8)	0.0325 (8)	−0.0038 (8)
C15	0.0363 (8)	0.0439 (9)	0.0407 (8)	0.0005 (7)	0.0211 (7)	−0.0006 (7)
C16	0.0349 (8)	0.0403 (8)	0.0420 (8)	−0.0022 (6)	0.0206 (7)	−0.0005 (7)
C17	0.0409 (9)	0.0596 (10)	0.0455 (9)	0.0058 (7)	0.0220 (7)	0.0009 (8)
C18	0.0576 (11)	0.0638 (11)	0.0452 (9)	0.0006 (9)	0.0276 (8)	−0.0052 (8)
C19	0.0502 (10)	0.0636 (11)	0.0412 (9)	−0.0057 (8)	0.0167 (8)	0.0005 (8)
N4	0.0426 (8)	0.0701 (10)	0.0471 (8)	0.0048 (7)	0.0173 (7)	0.0048 (7)

Geometric parameters (Å, º)

N1—C7	1.3253 (16)	C8—C9	1.4823 (19)
N1—C15	1.3440 (18)	C9—C14	1.379 (2)
N2—C8	1.3356 (19)	C9—C10	1.381 (2)
N2—N3	1.3448 (17)	C10—C11	1.383 (2)
N3—C15	1.3322 (18)	C10—H10A	0.9300
C20—N4	1.3313 (18)	C11—C12	1.375 (2)
C20—C16	1.385 (2)	C11—H11A	0.9300

C20—H20A	0.9300	C12—C13	1.363 (2)
C1—C6	1.385 (2)	C12—H12A	0.9300
C1—C2	1.388 (2)	C13—C14	1.386 (2)
C1—H1B	0.9300	C13—H13A	0.9300
C2—C3	1.375 (2)	C14—H14A	0.9300
C2—H2B	0.9300	C15—C16	1.4788 (19)
C3—C4	1.370 (2)	C16—C17	1.386 (2)
C3—H3B	0.9300	C17—C18	1.377 (2)
C4—C5	1.381 (2)	C17—H17A	0.9300
C4—H4B	0.9300	C18—C19	1.371 (2)
C5—C6	1.386 (2)	C18—H18A	0.9300
C5—H5A	0.9300	C19—N4	1.335 (2)
C6—C7	1.4887 (19)	C19—H19A	0.9300
C7—C8	1.4126 (19)		

C7—N1—C15	116.31 (12)	C10—C9—C8	120.64 (13)
C8—N2—N3	119.33 (12)	C9—C10—C11	120.51 (15)
C15—N3—N2	118.20 (13)	C9—C10—H10A	119.7
N4—C20—C16	124.33 (15)	C11—C10—H10A	119.7
N4—C20—H20A	117.8	C12—C11—C10	120.12 (17)
C16—C20—H20A	117.8	C12—C11—H11A	119.9
C6—C1—C2	119.60 (16)	C10—C11—H11A	119.9
C6—C1—H1B	120.2	C13—C12—C11	119.82 (15)
C2—C1—H1B	120.2	C13—C12—H12A	120.1
C3—C2—C1	120.50 (16)	C11—C12—H12A	120.1
C3—C2—H2B	119.8	C12—C13—C14	120.27 (15)
C1—C2—H2B	119.8	C12—C13—H13A	119.9
C4—C3—C2	119.95 (16)	C14—C13—H13A	119.9
C4—C3—H3B	120.0	C9—C14—C13	120.54 (16)
C2—C3—H3B	120.0	C9—C14—H14A	119.7
C3—C4—C5	120.19 (16)	C13—C14—H14A	119.7
C3—C4—H4B	119.9	N3—C15—N1	125.41 (13)
C5—C4—H4B	119.9	N3—C15—C16	117.45 (13)
C4—C5—C6	120.33 (15)	N1—C15—C16	117.13 (12)
C4—C5—H5A	119.8	C20—C16—C17	117.00 (13)
C6—C5—H5A	119.8	C20—C16—C15	121.79 (13)
C1—C6—C5	119.42 (14)	C17—C16—C15	121.21 (13)
C1—C6—C7	120.15 (13)	C18—C17—C16	119.76 (15)
C5—C6—C7	120.41 (13)	C18—C17—H17A	120.1
N1—C7—C8	120.00 (13)	C16—C17—H17A	120.1
N1—C7—C6	117.05 (12)	C19—C18—C17	118.28 (15)
C8—C7—C6	122.95 (12)	C19—C18—H18A	120.9
N2—C8—C7	120.14 (13)	C17—C18—H18A	120.9
N2—C8—C9	116.00 (13)	N4—C19—C18	123.81 (15)
C7—C8—C9	123.86 (13)	N4—C19—H19A	118.1
C14—C9—C10	118.71 (14)	C18—C19—H19A	118.1
C14—C9—C8	120.64 (14)	C20—N4—C19	116.80 (14)

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the N4,C16–C20 and C1–C6 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20*A*···N3	0.93	2.49	2.824 (4)	102
C13—H13*A*···*Cg*1^{i}	0.93	3.49	3.345 (4)	91
C19—H19*A*···*Cg*2^{ii}	0.93	3.67	3.109 (4)	121

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1.