

## 5,6-Diphenyl-3-(pyrazin-2-yl)-1,2,4-triazine

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## Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$   
R factor = 0.039  
wR factor = 0.108  
Data-to-parameter ratio = 15.1

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

The title compound,  $\text{C}_{38}\text{H}_{26}\text{N}_{10}$ , has been structurally characterized. The molecule contains two heterocycles that are almost coplanar.

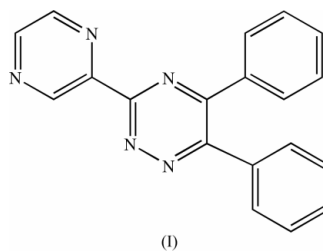
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## Comment

Ruthenium(II) polypyridyl complexes have aroused intense interest because of their extensive applications in the fields of photochemistry, photophysics, photocatalysis, electrochemistry and biochemistry. In particular, their important applications for DNA binding, electrochemical luminescence and solar-energy battery materials are well known (Juris *et al.*, 1988; Krausz & Riesen, 1997; MacDonnell *et al.*, 1999). The interactions of polypyridylruthenium complexes with DNA have been well documented (Barton & Lolis, 1985; Barton, 1986; Ambroize & Maiya, 2000). In our group, we have focused our interest on an investigation of the mechanism of their interaction with DNA; many new substituted derivatives of the ligands of ruthenium(II) polypyridyl complexes have been designed and synthesized (Liu *et al.*, 2001; Xiong & Ji, 1999; Ji *et al.*, 2001; Wu *et al.*, 1997). However, it is noteworthy that most of these ligands are symmetric and that the use of asymmetric ligands for coordination is rare. We are interested in the investigation of polypyridylruthenium(II) complexes with asymmetric ligands as DNA binding reagents. In this report, we discuss the crystal structure analysis of the asymmetric ligand 5,6-diphenyl-3-(pyrazin-2-yl)-1,2,4-triazine, (I).



The C–N distances show no remarkable features, with values in the range 1.326 (2)–1.344 (2) Å, which are shorter than the single-bond length of 1.480 Å and longer than the typical C=N distance of 1.280 Å, indicating partial double-bond character and suggesting conjugation in the heterocycle. The C6–C8, C4–C5 and C7–C14 bond lengths are all close to the standard values for single bonds between trigonally linked C atoms (Cruickshank & Spark, 1960). The two heterocycles in the solid structure are almost coplanar, with a dihedral angle of 1.97 (8)°.

## Experimental

The title compound was synthesized using the method described in the literature (Case, 1968). The single crystal used for X-ray analysis was recrystallized from ethanol. Elemental analysis calculated for  $C_{19}H_{13}N_5$  (%): C 73.31, H 4.18, N 22.51; found: 73.06, H 4.31, N 22.38.

### Crystal data

$C_{19}H_{13}N_5$	$D_x = 1.360 \text{ Mg m}^{-3}$
$M_r = 311.34$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 4369 reflections
$a = 14.294 (7) \text{ \AA}$	$\theta = 1.7\text{--}27.1^\circ$
$b = 7.027 (4) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 15.679 (8) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 105.149 (9)^\circ$	Block, yellow
$V = 1520.2 (13) \text{ \AA}^3$	$0.50 \times 0.30 \times 0.28 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART CCD diffractometer	3290 independent reflections
$\varphi$ and $\omega$ scans	2397 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (Blessing, 1995)	$R_{\text{int}} = 0.022$
$T_{\text{min}} = 0.959$ , $T_{\text{max}} = 0.977$	$\theta_{\text{max}} = 27.1^\circ$
9062 measured reflections	$h = -18 \rightarrow 18$
	$k = -8 \rightarrow 8$
	$l = -13 \rightarrow 20$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.3681P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.108$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
3290 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
218 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0224 (17)

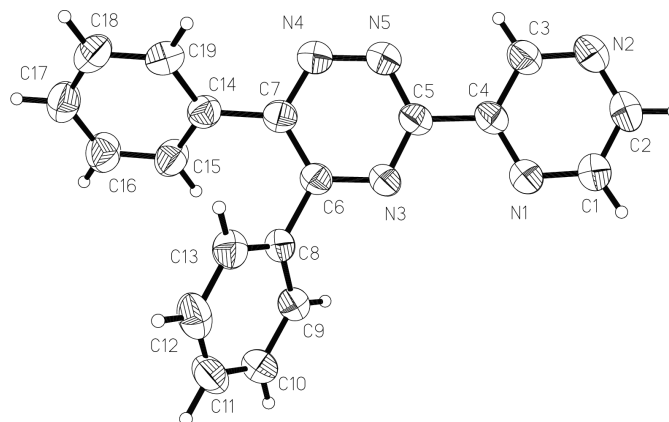
**Table 1**

Selected geometric parameters ( $\text{\AA}$ ).

N1—C1	1.334 (2)	N5—C7	1.327 (2)
N1—C4	1.337 (2)	N5—C5	1.344 (2)
N2—C3	1.328 (2)	C4—C5	1.489 (2)
N2—C2	1.331 (2)	C6—C8	1.481 (2)
N3—C5	1.333 (2)	C7—C14	1.489 (2)
N4—C6	1.339 (2)		

H atoms were placed in calculated positions and refined using a riding model.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.



**Figure 1**

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

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## References

- Ambroize, A. & Maiya, B. G. (2000). *Inorg. Chem.* **39**, 4264–4272.
- Barton, J. K. (1986). *Science*, **233**, 727–734.
- Barton, J. K. & Lolis, E. (1985). *J. Am. Chem. Soc.* **107**, 708–709.
- Blessing, R. H. (1995). *Acta Cryst. A* **51**, 33–38.
- Bruker (1998). *SMART* (Version 5.0) and *SHELXTL* (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1999). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Case, F. H. (1968). *J. Heterocycl. Chem.* **5**, 223–226.
- Cruickshank, D. W. J. & Spark, R. A. (1960). *Proc. R. Soc. A*, **258**, 270–285.
- Ji, L. N., Zou, X. H. & Liu, J. G. (2001). *Coord. Chem. Rev.* **216**, 513–536.
- Juris, A., Balzani, V., Barigelli, F., Campagna, S., Belser, P. & von Zelewsky, A. (1988). *Coord. Chem. Rev.* **84**, 85–277.
- Krausz, E. & Riesen, H. (1997). *Coord. Chem. Rev.* **159**, 9–40.
- Liu, J. G., Zhang, Q. L., Shi, X. F. & Ji, L. N. (2001). *Inorg. Chem.* **40**, 5045–5050.
- MacDonnell, F. M., Kim, M. J. & Bodge, S. (1999). *Coord. Chem. Rev.* **186**, 535–549.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Wu, J. Z., Ye, B. H., Wang, L., Ji, L. N., Zhou, J. Y., Li, R. H. & Zhou, Z. Y. (1997). *J. Chem. Soc. Dalton Trans.* pp. 1395–1401.
- Xiong, Y. & Ji, L. N. (1999). *Coord. Chem. Rev.* **186**, 711–733.