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2,3,7,8-Tetrakis(2-pyridyl)pyrazino[2,3-*g*]quinoxaline

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The title compound, $C_{30}H_{18}N_8$, is a crystallographically centrosymmetric molecule. The pyrazine ring makes dihedral angles of 43.6 (3) and 33.0 (2)° with the two independent pyridine rings, and the dihedral angle between the two pyridine rings is 58.3 (3)°. The favoured orientation of the pyridine rings is such that their N atoms face each other.

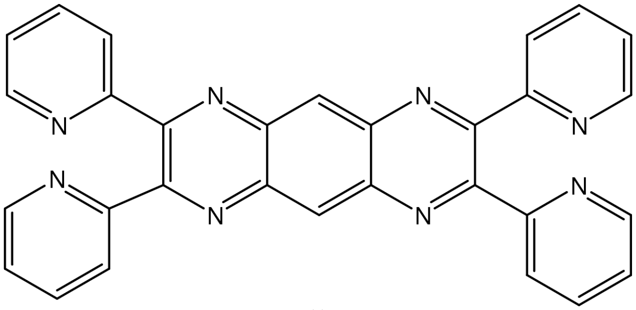
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.104
Data-to-parameter ratio = 11.8

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

Comment

Bridging polypyridyl ligands have been actively studied in recent years as building blocks for supramolecular assemblies (Hagrman *et al.*, 1999; Leininger *et al.*, 2000). Some of the polypyridyl compounds are of considerable interest because of the potential functionality of their metal complexes as photonic molecular devices (Eggleston *et al.*, 1997; Miller *et al.*, 1999) and DNA probes (Yam *et al.*, 1995; Holmlin *et al.*, 1999). Incorporating a ligand with two chelating sites into the coordination sphere allows systematic construction of large supramolecular assemblies capable of acting as antennae in energy-conversion schemes, where the photochemical and redox properties of the complexes are strongly dependent on the nature of the ligands (Waterland *et al.*, 2000). Since the stereochemistry of such compounds is so useful in the rational design of new functional materials, we report herein the crystal structure of 2,3,7,8-tetrakis(2-pyridyl)pyrazino[2,3-*g*]-quinoxaline, (I). In this structure, there is half a molecule in the asymmetric unit and the other half is inversion-related.



(I)

A perspective view of the title compound including the atomic numbering scheme is shown in Fig. 1. It consists of a pyrazino[2,3-*g*]quinoxaline system substituted with four pyridine rings. The two independent pyridine rings are not coplanar with each other nor with the pyrazine ring due to steric clashes between the H atoms of the pyridine rings. The torsion angle between the C—C bonds connecting the pyridine rings to the pyrazine ring (C5—C6—C7—C8) is 19.4 (3)°.

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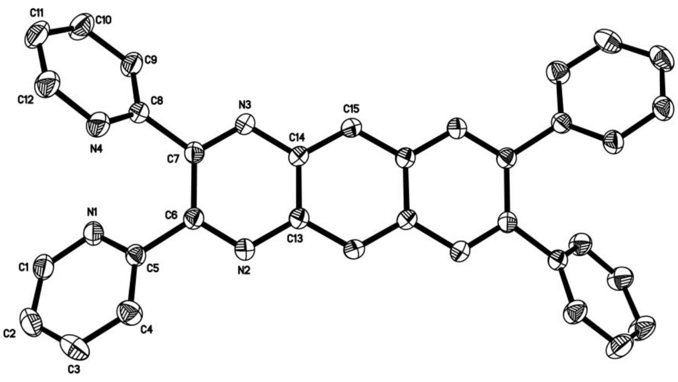

Figure 1
The molecular structure of (I) showing 30% probability displacement ellipsoids. H atoms have been omitted.

The pyrazine ring makes dihedral angles of 43.6 (3) and 33.0 (2)° with the two independent pyridine rings. The dihedral angle between the two pyridine rings is 58.3 (3)° and their N atoms face each other. In the central C_6 ring and the pyrazine ring, the mean deviation of any atom from the best-fit planes describing them are 0.0046 (1) and 0.0369 (3) Å, respectively. Furthermore, all non-H atoms in the pyrazino[2,3-*g*]quinoxaline system lie roughly in a plane: the mean deviation of any non-H atoms from the best-fit plane describing them is 0.0522 (2) Å. These distortions from planarity in the molecule are similar to those in its analogues (Rasmussen *et al.*, 1990; Du *et al.*, 2001). The C—N bond distances lie in the range 1.306 (3)–1.382 (2) Å and are significantly shorter than normal C—N single bonds (1.47 Å; Sasada, 1984) and longer than the C═N double-bond distance (1.28 Å; Wang *et al.*, 1998) due to the π-electron repulsion of the system. The C—C bond distances are in the range 1.367 (4)–1.489 (3) Å and all the bond angles are about 120°, falling within normal limits. There are no hydrogen bonds or π–π-stacking interactions between different molecules in the unit cell.

Experimental

The title compound was synthesized by the reaction of 1,2,4,5-benzenetetramine and 2,2′-bipyridyl in a 1:2 molar ratio. Single crystals suitable for X-ray diffraction were obtained by slow diffusion of diethyl ether into a CH_2Cl_2/CH_3OH solution of the compound. The product was characterized by NMR and mass spectrometry, giving results consistent with those in the literature (Rillema & Mack, 1982).

Crystal data

$C_{30}H_{18}N_8$
$M_r = 490.52$
Monoclinic, $P2/c$
$a = 15.061$ (5) Å
$b = 6.2184$ (19) Å
$c = 13.908$ (4) Å
$\beta = 114.398$ (5)°
$V = 1186.3$ (6) Å^3
$Z = 2$
$D_x = 1.373$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4465 reflections
$\theta = 1.5$–25.0°
$\mu = 0.09$ mm^{-1}
$T = 298$ (2) K
Prism, yellow
0.20 × 0.20 × 0.15 mm

Data collection

Bruker SMART 1000 diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.983$, $T_{\max} = 0.987$
4515 measured reflections
2046 independent reflections
1217 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.035$
$\theta_{\max} = 25.0°$
$h = -17 \rightarrow 17$
$k = -3 \rightarrow 7$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.104$
$S = 0.94$
2046 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.008$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0092 (15)

Table 1
Selected geometric parameters (Å, °).

N1—C5	1.335 (3)	N3—C7	1.307 (3)
N1—C1	1.339 (3)	N3—C14	1.382 (2)
N2—C6	1.306 (3)	N4—C12	1.335 (3)
N2—C13	1.375 (2)	N4—C8	1.338 (3)
C5—N1—C1	116.6 (2)	N2—C6—C5	116.03 (19)
C6—N2—C13	118.11 (18)	N3—C7—C8	114.82 (18)
C7—N3—C14	118.25 (18)	N4—C8—C9	123.10 (19)
C12—N4—C8	116.4 (2)	N4—C8—C7	115.70 (19)
N1—C5—C6	116.48 (19)	C15—C14—N3	119.82 (19)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998).

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