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Key indicators

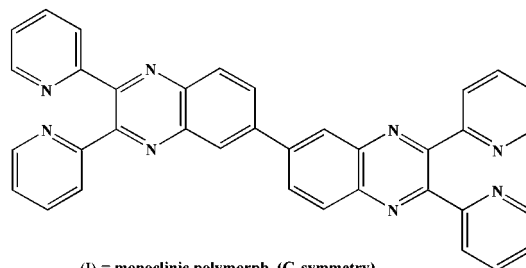
Single-crystal X-ray study
 $T = 223\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.042
 wR factor = 0.096
Data-to-parameter ratio = 13.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.A monoclinic polymorph of 2,3,2',3'-
tetrakis(2-pyridyl)-6,6'-biquinoxalinyll

When recrystallized from ethanol, the title compound, $\text{C}_{36}\text{H}_{22}\text{N}_8$, crystallized in the monoclinic space group $P2_1/n$, with the molecule located on an inversion center. The quinoxaline moiety is approximately planar and is coplanar with the symmetry-related moiety in the molecule. The two pyridine substituents lie out of the plane of the quinoxaline moiety by $40.1(1)$ and $42.3(1)^\circ$. They are inclined to one another by $56.8(2)^\circ$, with their N atoms on opposite sides of the mean plane through the quinoxaline moiety.

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Comment

The use of bridging polypyridyl ligands in the construction of coordination polymers is of particular interest in regard to their macroscopic properties. The development of synthetic strategies to form novel two- and three-dimensional networks is a rapidly expanding field in crystal engineering, as such compounds may have potential applications in many areas, such as molecular magnetism (Marioni *et al.*, 1986; Graf *et al.*, 1997), electrochemistry (Rillema *et al.*, 1982) and their use as host compounds for a variety of guest molecules (Moulton & Zaworotko, 2001). The choice of the metal bridging ligand is of fundamental importance in designing functional materials.



(I) = monoclinic polymorph (C_1 symmetry)
(II) = orthorhombic polymorph (C_2 symmetry)

The title compound, (I), was first synthesized by Rillema *et al.* (1982), who studied the electrochemistry of a series of compounds containing one, two, three and four ruthenium bis(bipyridine) units bound to (I). When recrystallized from water/methanol, an orthorhombic polymorph, (II), was obtained (Neels & Stoeckli-Evans, 2003). When recrystallized from ethanol, a monoclinic polymorph was obtained, in space group $P2_1/n$, with an inversion center within the molecule (Fig. 1). The bond distances and angles in the entire molecule of (I) are as expected. They can be compared with those observed in other 2,3-bis(*C*-substituted) quinoxalines, such as 2,3-bis(2-pyridyl)quinoxaline (Rasmussen *et al.*, 1990; Goodwin *et al.*, 1990). The quinoxaline moiety is approximately planar, the dihedral angle between planes *C* and *D* being $5.0(1)^\circ$. The largest deviation of any atom from the

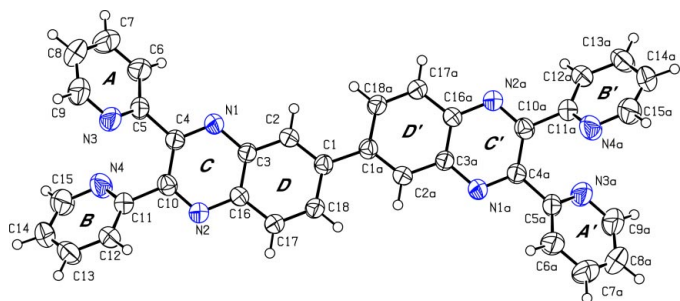


Figure 1

A perspective view of the monoclinic polymorph (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. [Symmetry code for a : $-x, 1 - y, -z$.]

least-squares plane is 0.082 (3) Å. The two symmetry-related quinoxaline moieties are coplanar and the two independent pyridine rings (*A* and *B*) are twisted out of the plane of the quinoxaline unit. The dihedral angle between the pyridine rings themselves is 56.8 (2)°. The N atoms face one another, but are directed above and below the plane of the molecule. Pyridine rings *A* and *B* are inclined to the mean plane through the quinoxaline moiety by 40.1 (1) and 42.3 (1)°, respectively. The pyrazine ring is also distorted, as in the above mentioned compounds, the N1–C4–C10–N2 and N1–C3–C16–N2 torsion angles being 9.8 (4)° and 8.0 (4)°, respectively.

In the crystal structure, symmetry-related molecules are linked by a C–H···N interaction, resulting in the formation of a hydrogen-bonded zigzag polymer extending in the c direction (Table 1). There is one C–H··· π interaction [C12–H12···Cg1; Cg1 is the centroid of ring *D*(1 + x, y, z); Table 1].

Experimental

Compound (I) was synthesized by the condensation reaction of biphenyl-3,4,3',4'-tetraamine with 2,2'-bipyridyl in a 1:2 molar ratio (Rillema *et al.*, 1982). Thin orange plate-like crystals, suitable for X-ray diffraction, were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{36}H_{22}N_8$
 $M_r = 566.62$
 Monoclinic, $P2_1/n$
 $a = 6.8892$ (6) Å
 $b = 7.7255$ (6) Å
 $c = 26.895$ (2) Å
 $\beta = 97.024$ (11)°
 $V = 1420.7$ (2) Å³
 $Z = 2$

$D_x = 1.325$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 2327 reflections
 $\theta = 2.3$ – 25.9 °
 $\mu = 0.08$ mm⁻¹
 $T = 223$ (2) K
 Plate, orange
 $0.35 \times 0.30 \times 0.10$ mm

Data collection

Stoe IPDS diffractometer
 φ scans
 10 763 measured reflections
 2771 independent reflections
 1024 reflections with $I > 2\sigma(I)$

$R_{int} = 0.133$
 $\theta_{max} = 25.9$ °
 $h = -8 \rightarrow 8$
 $k = -9 \rightarrow 9$
 $l = -32 \rightarrow 33$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.096$
 $S = 0.73$
 2771 reflections
 199 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0319P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.14$ e Å⁻³
 $\Delta\rho_{min} = -0.16$ e Å⁻³

Table 1

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C7–H7···N4 ⁱ	0.94	2.56	3.487 (4)	167
C12–H12···Cg1 ⁱⁱ	0.94	2.81	3.343 (3)	117

Symmetry codes: (i) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ii) $1 + x, y, z$. Cg1 is the centroid of ring *D*.

The crystals were thin plates and diffracted weakly. Only 37% of the data can be considered to be observed [$I > 2\sigma(I)$], which resulted in a relatively high R_{int} value and a low S value. H atoms were introduced in calculated positions and treated as riding atoms, with C–H = 0.94 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *EXPOSE* (Stoe, 2000); cell refinement: *CELL* (Stoe, 2000); data reduction: *INTEGRATE* (Stoe, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON99* (Spek, 1990); software used to prepare material for publication: *SHELXL97*.

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