

Bis[4-(3-pyridylmethyleneamino)-
phenyl]methaneQing Wang,^{a,b} Xiang-Dong Pi^c and Cheng-Yong Su^{a,b*}

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Received 22 November 2004

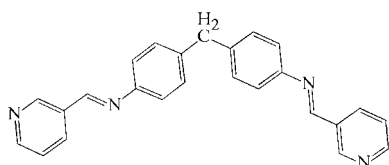
Accepted 9 December 2004

Online 15 January 2005

In the title Schiff base compound, C₂₅H₂₀N₄, the two rigid parts adopt an angular conformation, thus making the compound a potential non-linear ditopic ligand for the construction of interesting coordination polymers.

Comment

Rigid bipyridyl-type bidentate Schiff base ligands have been intensively utilized in order to assemble various coordination polymers with intriguing topology (Barnett & Champness, 2003; Su *et al.*, 2004), while angular chelating bipyridyl Schiff base ligands are known to form helical complexes (Guo *et al.*, 2002). However, angular ditopic Schiff base ligands containing non-chelating dipyridyl groups have rarely been used to



construct coordination assemblies. As a continuation of our study of the coordination chemistry of semi-rigid ligands (Su *et*

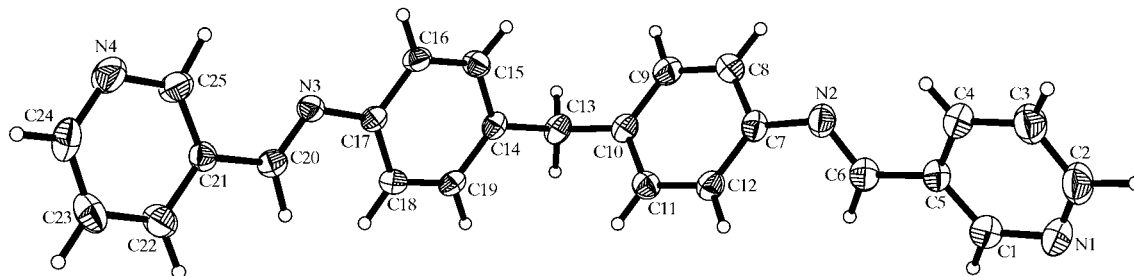


Figure 1

A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.

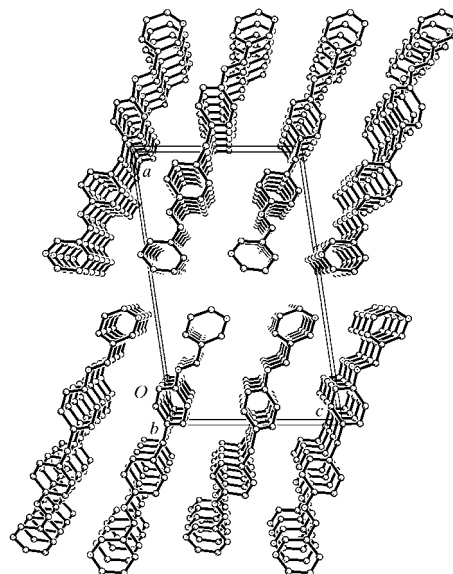


Figure 2

The molecular packing in (I), viewed along the *b* axis. H atoms have been omitted for clarity.

al., 2003; Chen *et al.*, 2002), we have synthesized the title compound, (I), and report its single-crystal structure.

Compound (I) crystallizes in the non-centrosymmetric space group *Pc*, which was confirmed by the ADDSYM check in *PLATON* (Spek, 1990, 2003). As expected, the two rigid parts incorporating the 3-pyridyl groups adopt an angular arrangement (Fig. 1). The dihedral angle between the two benzene rings linked by the methylene group is 77.95 (16)°, which determines the specific orientation of the pyridyl groups. However, the pyridyl rings are not exactly coplanar with the benzene rings, although the coplanar conformation is energetically preferred (Su *et al.*, 2000). On one side of the methylene group, the pyridyl (C21–C25/N4) and benzene (C14–C19) rings are nearly coplanar, with a dihedral angle of 9.95 (17)°, but on the other side, these two rings (the C7–C12 benzene and C1–C5/N1 pyridyl ring) adopt a dihedral angle of 53.86 (18)°, significantly deviating from the mean plane. Such asymmetric disposition of the two rigid branches may account for the absence of centrosymmetry in the crystal.

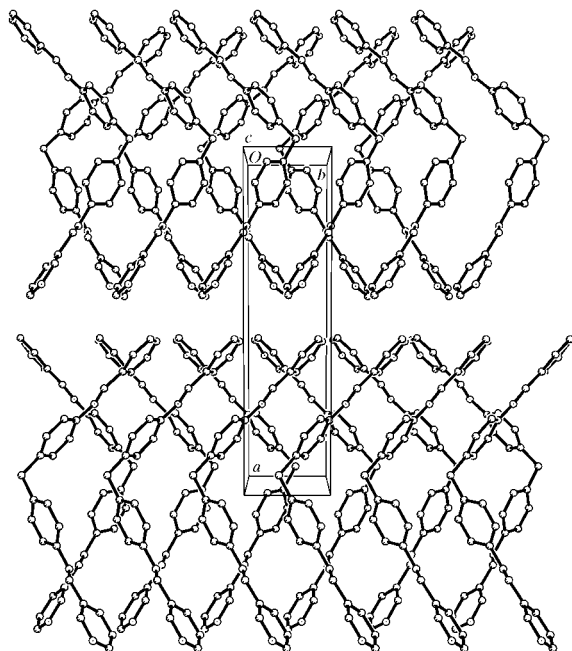


Figure 3
The molecular packing in (I), viewed along the *c* axis. H atoms have been omitted for clarity.

Analysis of the crystal-packing mode reveals that the ligands stack up in the crystal lattice with each six-membered ring (both benzene and pyridyl) parallel to its counterpart in adjacent ligands, giving a shortest centroid-to-centroid distance of *ca* 4.64 Å (corresponding to the length of the *b* axis). The overlapping arrangement of the ligands results in a one-dimensional array along the *b* axis. Such arrays are aligned parallel to each other, forming two-dimensional layers along the *c* axis (Fig. 3).

Experimental

The title compound was prepared from 4,4'-methylenedianiline and 3-pyridinecarboxaldehyde. Single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{25}H_{20}N_4$
 $M_r = 376.45$
Monoclinic, *Pc*
 $a = 18.751$ (5) Å
 $b = 4.641$ (2) Å
 $c = 11.387$ (11) Å
 $\beta = 98.394$ (19)°
 $V = 980.3$ (2) Å³
 $Z = 2$
 $D_x = 1.275$ Mg m⁻³

Mo *K*α radiation
Cell parameters from 25 reflections
 $\theta = 8$ –17.6°
 $\mu = 0.08$ mm⁻¹
 $T = 293$ (2) K
Block, yellow
0.4 × 0.35 × 0.26 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.956$, $T_{\max} = 0.980$
3793 measured reflections
1920 independent reflections
1287 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$
 $\theta_{\text{max}} = 26^\circ$
 $h = -23 \rightarrow 22$
 $k = -5 \rightarrow 5$
 $l = 0 \rightarrow 14$
2 standard reflections
every 3600 reflections
intensity decay: <1%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.071$
 $S = 1.02$
1920 reflections
343 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.031P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.11$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.10$ e Å⁻³
Extinction correction: *SHELXTL*
Extinction coefficient: 0.028 (4)

All H atoms were initially located in a difference Fourier map and were refined freely along with an isotropic displacement parameter. No Friedel pairs were measured and, as expected, the Flack (1983) parameter was indeterminate.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXTL* (Bruker, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China and the Natural Science Foundation of Guangdong Province for financial support.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: HJ1037). Services for accessing these data are described at the back of the journal.

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