continuous support of the DNA molecular recognition project, and Mike Eaton and Jim Turner for helpful discussions.

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Knowledge of the solid-state structure of this ligand will enable further understanding of its chemical behaviour and coordination ability.

dmbp
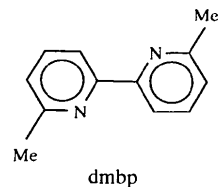
The molecule crystallizes in the space group $P2_1/c$, lying on a centre of symmetry, with the N atoms of the pyridyl rings *trans* to each other around the central bond. This conformation of the uncoordinated molecule contrasts with the *cisoid* arrangement necessary when it acts as a chelating ligand. The molecule is planar, with only the methyl H atoms deviating significantly from the plane. Bond lengths and angles are as expected for this type of system and compare favourably with those reported for other bipyridyl molecules (Nakatsu *et al.*, 1972; Troyanov *et al.*, 1989).

6,6'-Dimethyl-2,2'-bipyridyl

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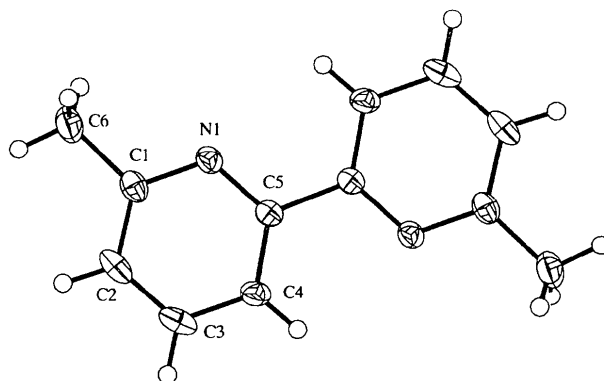
Abstract

In the solid state, the novel ligand 6,6'-dimethyl-2,2'-bipyridyl (dmbp), $C_{12}H_{12}N_2$, is a planar centrosymmetric molecule in which the pyridyl N atoms have a *transoid* arrangement, by virtue of the symmetry.

Comment

Square-planar complexes of Pt^{II} containing the title dmbp ligand, *e.g.* [Pt(dmbp)Cl₂], have aroused much interest recently due to their unusual redox and physical properties (Zuleta *et al.*, 1990; Miskowski *et al.*, 1993).

Fig. 1. The molecular structure of dmbp shown with 50% probability ellipsoids.

Experimental

The title compound was prepared according to the method of Badger & Sasse (1956, 1963), with modifications (Case, 1966; Burstal, 1938; Parks *et al.*, 1973; Newcome *et al.*, 1981; Rodde & Breitmaier, 1987) in order to improve yield. 2-Picoline (Aldrich) was refluxed (96 h) over freshly degassed Raney-nickel catalyst (dried under vacuum for 3 h) using a Soxhlet apparatus. NaOH was added to the alloy at 353–363 K over a period of 15 min. After removal of unreacted 2-picoline by distillation, the crude product was dissolved in ethanol, heated to boiling point and filtered over decolourising charcoal. The resulting yellow solution was evaporated to dryness and sublimed at 373 K. Recrystallization from ethanol produced clear prismatic crystals, which were characterized by NMR using a Bruker AMX360 (DMSO-d_6): δ 2.52 (s, py-CH₃, 6H), 7.25 (d, 5,5'-py-H, J = 7.5 Hz, 2H), 7.76 (t, 4,4'-py-H, J = 7.7 Hz, 2H) and 8.14 (d, 3,3'-py-H, J = 7.8 Hz, 2H).

Crystal data

$C_{12}H_{12}N_2$
$M_r = 184.24$
Monoclinic
$P2_1/c$
$a = 6.775\,(5)$ Å
$b = 11.146\,(3)$ Å
$c = 7.055\,(4)$ Å
$\beta = 111.72\,(6)°$
$V = 494.9\,(4)$ Å^3
$Z = 2$
$D_x = 1.241$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 50
reflections
$\theta = 3.24–24.89°$
$\mu = 0.075$ mm^{-1}
$T = 150\,(2)$ K
Prism
$0.35 \times 0.32 \times 0.11$ mm
Colourless

Data collection

Delft Instruments FAST-TV
area-detector diffractom-
eter
Scan method: Darr
et al. (1993)
Absorption correction: none
1612 measured reflections
742 independent reflections

613 reflections with
$I > 2\sigma(I)$
$R_{int} = 0.100$
$\theta_{max} = 24.89°$
$h = -7 \rightarrow 8$
$k = -12 \rightarrow 6$
$l = -8 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.135$
$S = 1.065$
742 reflections
65 parameters
H atoms riding
$w = 1/[\sigma^2(F_o^2) + (0.0766P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.010$
$\Delta\rho_{max} = 0.213$ e Å^{-3}
$\Delta\rho_{min} = -0.266$ e Å^{-3}
Extinction correction: none
Scattering factors from
*International Tables for
Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

N1—C1	1.338 (2)	C2—C3	1.383 (3)
N1—C5	1.353 (2)	C3—C4	1.377 (2)
C1—C2	1.390 (3)	C4—C5	1.386 (2)
C1—C6	1.503 (3)	C5—C5^i	1.485 (3)
C1—N1—C5	118.37 (15)	C4—C3—C2	118.94 (18)
N1—C1—C2	122.28 (16)	C3—C4—C5	119.26 (16)
N1—C1—C6	116.12 (18)	N1—C5—C4	122.08 (15)
C2—C1—C6	121.60 (17)	N1—C5—C5^i	116.50 (18)
C3—C2—C1	119.06 (17)	C4—C5—C5^i	121.41 (17)

Symmetry code: (i) $-x, 2 - y, -z$.

The absence of any intensity decay was confirmed by compar-
ing intensities of equivalent reflections at the beginning and
end of data collection. The methyl groups were allowed tor-
sional freedom during the course of the refinement. H atoms
were included in calculated positions (riding model), with U_{iso}
set at 1.2 (CH) and 1.5 (CH$_3$) times the U_{eq} of the parent
atoms.

Data collection: *MADNES* (Pflugrath & Messerschmidt,
1989). Cell refinement: *REFINE* in *MADNES*. Data reduction:
ABSMAD (Karaulov, 1992). Program(s) used to solve struc-
ture: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine
structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics:
SNOOPI (Davies, 1983). Software used to prepare material
for publication: *SHELXL*93.

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5,15-Bis(3,5-di-*tert*-butylphenyl)-10,20-bis-(trimethylsilylethynyl)porphyrin

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Abstract

In the title compound, $C_{58}H_{70}N_4Si_2$, the acetylene
groups lie in the plane of the porphyrin π system. The
angle between the plane of each phenyl ring and the
plane of the porphyrin is 62.39 (4)°. There are no $\pi-\pi$

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