O1—Li—O5	111 (1)	P1—C1*A*—C1*B*	120.3 (7)
O1—Li—O6	108 (2)	P1—C1*A*—C1*F*	121.7 (8)
O1—Li—O7	104 (2)	P1—C2*A*—C2*B*	121.6 (8)
O5—Li—O6	113 (1)	P1—C2*A*—C2*F*	119.7 (8)
O5—Li—O7	115 (1)		

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

The structure was solved by the Patterson method and refined by full-matrix least squares. Anisotropic displacement parameters were refined for all non-H atoms with the exception of 12 thf methylene C atoms. The large isotropic *B* values for these atoms (Table 1) and the large range shown by thf C—C bonds may indicate some disorder of the thf groups. All calculations were performed using the *SDP* system (Enraf–Nonius, 1985) on a MicroVAX II computer.

We thank the Hong Kong Research Grant Council and the University of Hong Kong for support.

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: MU1093). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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trans-Dichlorotetrapyridineruthenium(II)

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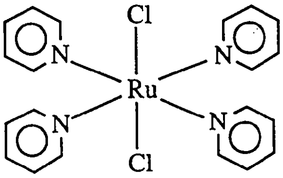
Abstract

$[Ru(py)_4Cl_2]$ (where py = pyridine, C_5H_5N), crystallizes in the tetragonal space group $I4_1/acd$. Ru and Cl atoms occupy sites of 222 and 2 point symmetry, respectively. The Ru atom has slightly distorted octahedral coordination. The Cl—Ru—Cl moiety is linear, as a result of symmetry requirements.

Comment

The title compound, (I), was prepared using a modification of procedures described by Bottomley & Mukaida (1982) and Gilbert, Rose & Wilkinson (1970). Hydrated $RuCl_3$ was dissolved in 90% ethanol. To this solution excess pyridine was added and the mixture was refluxed for 1 h. After cooling, the resulting precipitate was filtered and washed with water, and then with diethyl ether (yield 42%). Orange–red crystals suitable for X-ray analysis were grown by slow evaporation of a 1:1 CH_2Cl_2/CH_3CN solution of the complex.



(I)

Since there have been relatively few structural studies of *trans*-dichlorotetraamineruthenium(II) species, we have determined the structure of the title compound. It crystallizes in $I4_1/acd$ (No. 142; origin taken at $\bar{1}$). The Ru atom lies on the special position with site symmety 222 [Wyckoff position 8(*b*)] and the Cl atom lies on a twofold axis [Wyckoff position 16(*f*)]. The pyridine ligand is in a general position and four symmetrically related pyridine ligands are bonded to each Ru atom. The Ru—Cl bond distance is comparable to those observed in other dichlororuthenium(II) complexes (Seal & Ray, 1984), but is significantly longer than those observed in $[Ru^{III}(py)_4Cl_2]^+$ (Al-Zamil *et al.*, 1982).

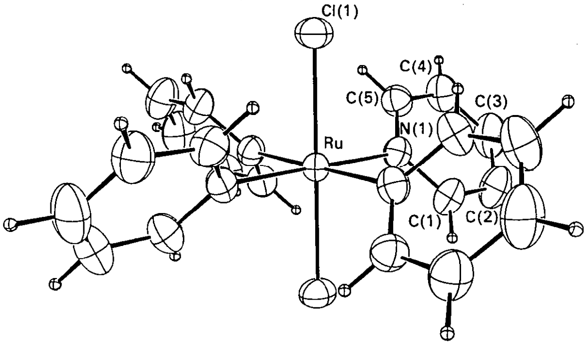


Fig. 1. The molecular structure of *trans*-$[Ru(py)_4Cl_2]$.

Experimental

Crystal data

$[Ru(C_5H_5N)_4Cl_2]$
$M_r = 488.38$
Tetragonal
$I4_1/acd$ (origin at $\bar{1}$)
$a = 15.701$ (2) Å
$c = 16.987$ (2) Å
$V = 4187.7$ (8) Å^3
$Z = 8$
$D_x = 1.550$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–13°
$\mu = 1.0$ mm^{-1}
$T = 293$ K
Block
0.22 × 0.12 × 0.12 mm
Orange–red

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: empirical
$T_{min} = 0.810$, $T_{max} = 0.999$
2293 measured reflections
1208 independent reflections

650 observed reflections $[F_o > 3\sigma(F_o)]$
$R_{int} = 0.022$
$\theta_{max} = 26°$
$h = 0 \rightarrow 19$
$k = 0 \rightarrow 19$
$l = 0 \rightarrow 20$
3 standard reflections
frequency: 120 min
intensity variation: ±2%

Refinement

Refinement on F
$R = 0.029$
$wR = 0.036$
$S = 1.119$
650 reflections
63 parameters
H-atom parameters not refined

$w = 4F_o^2/[\sigma^2(F_o^2) + (0.04F_o^2)^2]$
$(\Delta/\sigma)_{max} = 0.01$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Ru	0	1/4	1/8	2.249 (6)
Cl1	0.10837 (5)	$x+1/4$	1/8	3.50 (2)
N1	0.0659 (2)	0.1833 (2)	0.2115 (1)	2.70 (5)
C1	0.0251 (2)	0.1456 (2)	0.2720 (2)	3.45 (7)
C2	0.0676 (2)	0.1013 (3)	0.3299 (2)	4.40 (8)
C3	0.1541 (3)	0.0942 (3)	0.3267 (2)	4.86 (9)
C4	0.1964 (2)	0.1316 (2)	0.2653 (2)	3.91 (8)
C5	0.1507 (2)	0.1753 (2)	0.2093 (2)	3.18 (7)

Table 2. *Selected geometric parameters* (Å, °)

Ru—Cl1	2.4054 (6)	C1—C2	1.376 (5)
Ru—N1	2.079 (2)	C2—C3	1.363 (5)
N1—C1	1.347 (5)	C3—C4	1.369 (5)
N1—C5	1.337 (4)	C4—C5	1.373 (5)
Cl1—Ru—N1	90.23 (8)	C1—C2—C3	119.7 (3)
Ru—N1—C1	121.5 (2)	C2—C3—C4	118.6 (3)
Ru—N1—C5	121.5 (3)	C3—C4—C5	119.2 (3)
C1—N1—C5	116.9 (3)	N1—C5—C4	123.2 (3)
N1—C1—C2	122.5 (3)		

The space group $I4_1/acd$ was chosen from the systematic absences and led to a successful refinement. The structure was solved by the Patterson method and refined by full-matrix least squares. All calculations were performed using the *SDP* system (Enraf–Nonius, 1985) on a MicroVAX II computer.

We thank the Hong Kong Research Grant Council and the University of Hong Kong for support.

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: MU1092). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Sodium *trans*-Dicyano[*N*,*N*'-1,2-phenylenebis(2-pyridinecarboxamido)]cobaltate(III)

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Abstract

The Co atom in the $[Co^{III}(CN)_2(C_{18}H_{12}N_4O_2)]^-$ complex anion is hexacoordinate with a distorted octahedral geometry. The four N atoms in the amide ligand occupy equatorial positions and are coplanar to within 0.007 Å. The two CN groups are coordinated to Co in a *trans* configuration. The Na cation interacts with four complex anions through their cyanide-N and amide-O atoms, thereby adopting a distorted tetrahedral coordination.

Comment

We recently reported some σ-alkylcobalt(III) complexes bearing an organic amide ligand (bpb or bpc; see scheme below) (Mak, Wong, Yam, Lai & Che, 1991). We are also interested in the structural chemistry of coordination compounds containing these amide ligands. This study indicates that the bpb ligand in the $[Co(bpb)(CN)_2]^-$ anion (I) deviates from planarity; the interplanar angles between the

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