metal-organic papers

Bis(1,10-phenanthroline)[2-(2-pyridyl)-1H-benzimidazol-1-yl]ruthenium(II) perchlorate–toluene–acetonitrile (2/2/1)

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The Ru^{II} atom in the title complex, $[Ru(C_{12}H_8N_2)_2(C_{12}H_8N_3)]ClO_4 \cdot C_7H_8 \cdot 0.5CH_3CN$, is in a distorted octahedral environment coordinated by two 1,10-phenanthroline (phen) and one deprotonated 2-(2-pyridyl)benzimidazole (PIB) ligand.
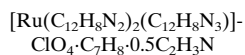
Comment

The ligand 2-(2-pyridyl)benzimidazole (PIBH) has been widely used in coordination chemistry (Harkins *et al.*, 1956; Chiswell *et al.*, 1964; Boca *et al.*, 1997; Shavaleev *et al.*, 2004). Many of the reported complexes have been of interest bacause deprotonation of the coordinated imidazoles can induce switching of the luminescence and redox properties (Haga, 1983; Haga *et al.*, 1991; Walter & Freiser, 1954).

(I)
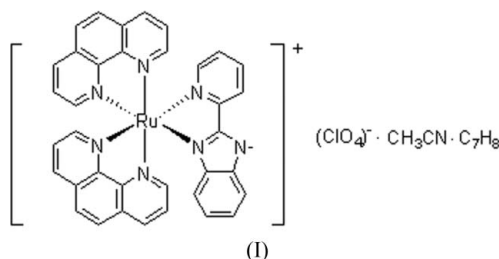
As part of an ongoing study of the properties of ruthenium(II) complexes containing PIBH (Liu *et al.*, 2006), we synthesized the title complex, $[Ru(phen)_2(PIB)](ClO_4) \cdot C_7H_8 \cdot 0.5CH_3CN$ [where PIB stands for the deprotonated 2-(2-pyridyl)benzimidazole and phen stands for 1,10-phenanthroline]. The title complex, (I), consists of an $[Ru(phen)_2(PIB)]^+$ cation, a ClO_4^- anion, one-half of an acetonitrile molecule and a toluene molecule. As shown in Fig. 1, the central Ru atom is chelated by two phen ligands and a PIB ligand. The coordination geometry about the Ru atom is distorted octahedral. The mean Ru—N bond length [2.070 (3) Å] is comparable with those of published ruthenium(II) complexes (Cambridge Structural Database, Version 5.26; Allen, 2002).

Experimental

2-(2-Pyridyl)benzimidazole(PIBH) (Walter & Freiser, 1954) and $[Ru(phen)_2(PIBH)](ClO_4)_2$ (Haga, 1983) were synthesized by procedures reported in the literature. A solution of $[Ru(phen)_2(PIBH)](ClO_4)_2$ (0.19 mmol, 0.172 g) in methanol (20 ml) was added to a sodium methoxide solution which was made *in situ* by dissolving sodium metal (0.72 mmol, 0.017 g) in methanol (10 ml). The color of the solution changed from red to dark red. The solution was heated with stirring for 30 min and then cooled to 273–278 K in a refrigerator. A deep-red microcrystalline solid was collected by filtration.

This was dissolved in acetonitrile and toluene (1:1 *v/v*) at room temperature. Several days later, deep-red single crystals of (I) suitable for X-ray analysis were obtained.

Crystal data

[Ru(C$_{12}$H$_8$N$_2$)$_2$(C$_{12}$H$_8$N$_3$)]- ClO$_4$·C$_7$H$_8$·0.5C$_2$H$_3$N	$V = 8016$ (6) Å^3
$M_r = 867.81$	$Z = 2$
Monoclinic, $C2/c$	$D_x = 1.438$ Mg m^{-3}
$a = 26.014$ (11) Å	Mo $K\alpha$ radiation
$b = 10.050$ (4) Å	$\mu = 0.51$ mm^{-1}
$c = 30.708$ (13) Å	$T = 298$ (2) K
$\beta = 93.223$ (7)°	Block, red
	$0.32 \times 0.26 \times 0.24$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	21776 measured reflections
φ and ω scans	7888 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	6398 reflections with $I > 2\sigma(I)$
$T_{min} = 0.854$, $T_{max} = 0.887$	$R_{int} = 0.031$
	$\theta_{max} = 26.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.052$	$+ 1.99P]$
$wR(F^2) = 0.140$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.28$	$(\Delta/\sigma)_{max} < 0.001$
7888 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
530 parameters	$\Delta\rho_{min} = -0.89$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

N1—Ru1	2.063 (3)	N4—Ru1	2.062 (3)
N2—Ru1	2.051 (3)	N5—Ru1	2.102 (3)
N3—Ru1	2.075 (3)	N6—Ru1	2.069 (3)
N2—Ru1—N4	174.78 (12)	N1—Ru1—N3	90.86 (13)
N2—Ru1—N1	79.98 (13)	N6—Ru1—N3	172.27 (12)
N4—Ru1—N1	95.56 (12)	N2—Ru1—N5	96.36 (12)
N2—Ru1—N6	88.98 (13)	N4—Ru1—N5	88.36 (11)
N4—Ru1—N6	94.13 (12)	N1—Ru1—N5	172.99 (13)
N1—Ru1—N6	94.86 (13)	N6—Ru1—N5	79.02 (13)
N2—Ru1—N3	97.15 (12)	N3—Ru1—N5	95.55 (12)
N4—Ru1—N3	80.12 (11)		

All H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with U_{iso}(H) = 1.2 or 1.5 U_{eq}(parent atom). Possible perchlorate disorder could not be satisfactorily modeled.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.
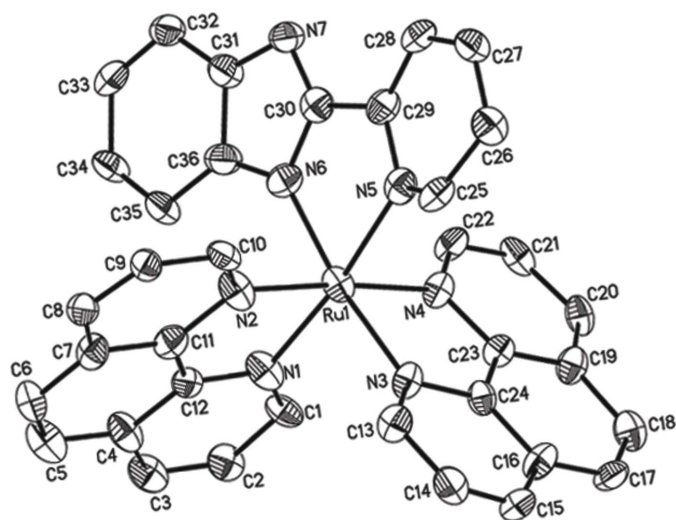
Figure 1
The molecular structure of the cation in (I), showing the atom-numbering scheme. Displacement ellipsoids are draw at the 30% probability level. H atoms have been omitted.
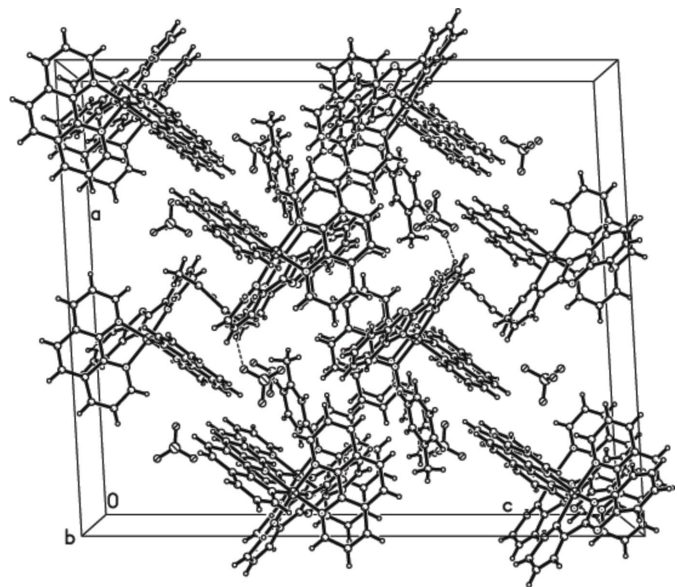

Figure 2
The crystal packing of the complex viewed down the *b* axis. The dashed lines indicate hydrogen bonds.

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