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Aqua(2,2′-bipyridine)(2,2′:6′,2″-terpyridine)-ruthenium(II) bis(perchlorate)

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Key indicators

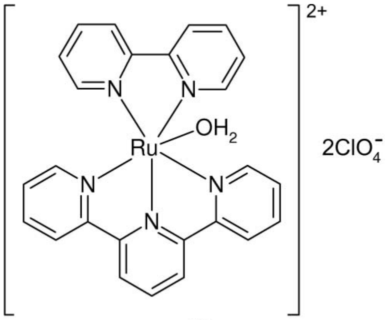
Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.007 Å
Disorder in solvent or counterion
R factor = 0.043
wR factor = 0.117
Data-to-parameter ratio = 13.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[Ru(C_{10}H_8N_2)(C_{15}H_{11}N_3)(H_2O)](ClO_4)_2$, two pairs of hydrogen bonds between the coordinated water molecules and perchlorate anions link the complexes into discrete $\{[(bipy)(terpy)Ru2O)](ClO_4)_2\}_2$ units (bipy = 2,2′-bipyridine and terpy = 2,2′:6′,2″-terpyridine).

Comment

Complexes of Ru^{II} with polypyridyl ligands are of interest on account of their photophysical and photochemical properties (Kalyanasundaram, 1982; Juris *et al.*, 1988). Like others (Yang *et al.*, 2005), we have used the cationic complex $[(bipy)(terpy)Ru(H_2O)]^{2+}$ (bipy = 2,2′-bipyridine and terpy = 2,2′:6′,2″-terpyridine) as the starting point for the preparation of more complex functional systems, and we report here the crystal structure of its perchlorate salt, (I).



(I)

The coordination geometry about Ru^{II} (Fig. 1 and Table 1) is distorted from octahedral on account of the limited bite angles of the polypyridyl ligands. The geometry of the complex is closely comparable to that of the reported PF_6^- salt (Yang *et al.*, 2005). One of the perchlorate anions is disordered over two orientations. In (I), the coordinated water molecules form hydrogen bonds to O atoms of the perchlorate anions (Table 2), generating discrete $\{[(bipy)(terpy)Ru(H_2O)](ClO_4)_2\}_2$ units (Fig. 2).

Experimental

Compound (I) was prepared according to a literature procedure (Takeuchi *et al.*, 1984). 0.05 g (0.07 mmol) of (I) was dissolved in THF/2,2,2-trifluoroethanol (2:1, 6 ml) and heated to boiling point. The solution was cooled to room temperature and $NaClO_4$ (0.05 g, 0.35 mmol) was added as a saturated aqueous solution (1 ml). Crystals of (I) were obtained by slow evaporation on standing under ambient conditions.

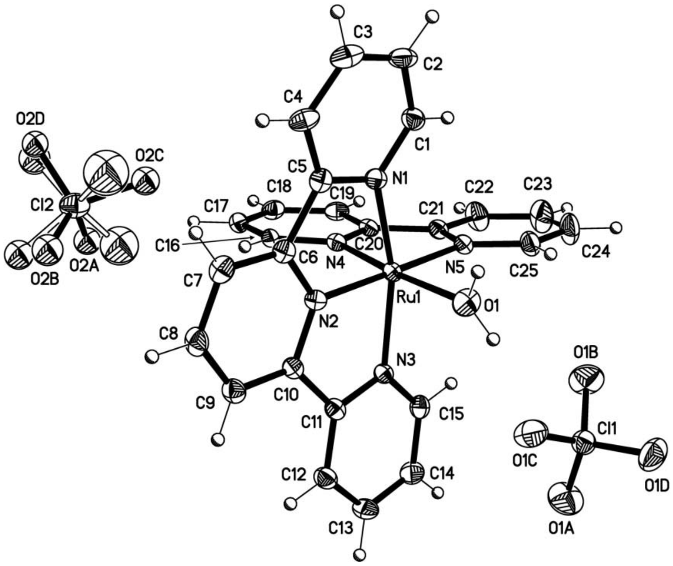


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level for non-H atoms. The two components of the disordered perchlorate anion are shown with solid and open bonds, respectively, and the O atoms are labelled for only one component.

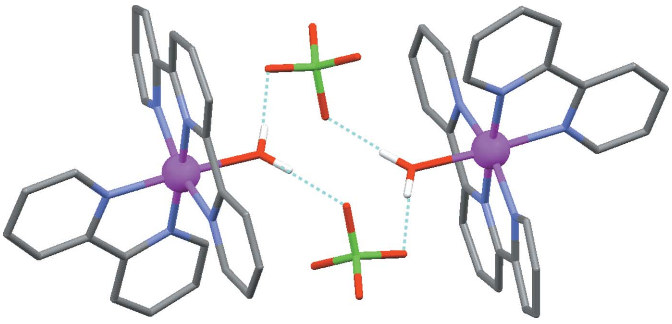


Figure 2
A discrete {[(bipy)(terpy)Ru(H_2O)](ClO_4)$_2$}$_2$ unit formed through O—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

Crystal data

[Ru($C_{10}H_8N_2$)($C_{15}H_{11}N_3$)-
(H_2O)](ClO_4)$_2$
M_r = 707.44
Orthorhombic, *Pbca*
a = 15.1483 (8) Å
b = 10.8842 (5) Å
c = 32.5725 (15) Å
V = 5370.5 (4) Å^3
Z = 8
Mo *K*α radiation
μ = 0.85 mm^{-1}
T = 180 (2) K
0.30 × 0.05 × 0.05 mm

Data collection

Bruker Nonius X8 APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.807, T_{max} = 0.959
48758 measured reflections
5070 independent reflections
3234 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.117
S = 1.03
5070 reflections
376 parameters
20 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ru1—N1	2.063 (4)	Ru1—N4	2.009 (4)
Ru1—N2	1.957 (4)	Ru1—N5	2.069 (4)
Ru1—N3	2.083 (4)	Ru1—O1	2.146 (3)
N1—Ru1—N2	79.35 (15)	N2—Ru1—O1	88.02 (14)
N1—Ru1—N3	158.70 (15)	N3—Ru1—N4	93.71 (14)
N1—Ru1—N4	92.21 (14)	N3—Ru1—N5	99.30 (14)
N1—Ru1—N5	101.93 (15)	N3—Ru1—O1	87.87 (13)
N1—Ru1—O1	88.28 (13)	N4—Ru1—N5	78.70 (15)
N2—Ru1—N3	79.59 (15)	N4—Ru1—O1	174.22 (14)
N2—Ru1—N4	97.73 (15)	N5—Ru1—O1	95.57 (14)
N2—Ru1—N5	176.21 (15)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1*C*	0.85	1.89	2.717 (5)	166
O1—H2···O1*D*^{i}	0.85	1.89	2.737 (5)	175

Symmetry code: (i) $-x+1, -y, -z+1$.

H atoms bound to C atoms were positioned geometrically, with C—H = 0.95 Å, and allowed to ride during subsequent refinement with U_{iso}(H) = 1.2U_{eq}(C). H atoms of the water molecule were visible in difference Fourier maps. Prior to refinement, the O—H distances were normalized to 0.85 Å, and the H atoms were allowed to ride on O1 with U_{iso}(H) = 1.5U_{eq}(O). One perchlorate anion (involved in O—H···O hydrogen bonding) is well ordered, while the second displays rotational disorder and is modelled as two components of equal site occupancy, with isotropic displacement parameters for the O atoms. The Cl—O distances in this anion were restrained to a common value [refined to 1.441 (3) Å] with a standard uncertainty of 0.01 Å, and the O···O distances were restrained to 1.633 times that value with a standard uncertainty of 0.02 Å.

Data collection: *APEX2* (Bruker–Nonius, 2004); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; 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*.

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