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Key indicators

Single-crystal X-ray study
T = 200 K
Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
Disorder in solvent or counterion
R factor = 0.058
wR factor = 0.155
Data-to-parameter ratio = 19.5

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

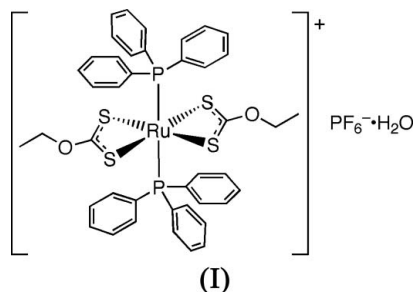
trans-Bis(*O*-ethylxanthato)bis(triphenyl- phosphine)ruthenium(III) hexafluorophosphate monohydrate

In the monoclinic crystal structure of the title compound, *trans*-[Ru(C₃H₅OS₂)₂(C₁₈H₁₅P)₂]PF₆·H₂O, the structure of the Ru^{III} complex cation is very similar to that in the orthorhombic crystal of the nonhydrated complex [Noda, Ohuchi, Hashimoto, Fujiki, Itoh, Iwatsuki, Noda, Suzuki, Kashiwabara & Takagi (2006), *Inorg. Chem.* **45**, 1349–1355]. In the present crystal structure, the P–Ru–P bond axes of the complex cations are aligned parallel to the [101] direction.

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Comment

Controlled-potential electrochemical oxidation of *cis*-[Ru^{II}(S₂COEt)₂(PPh₃)₂] in acetone in the presence of NH₄PF₆ afforded the corresponding ruthenium(III) complex, *trans*-[Ru^{III}(S₂COEt)₂(PPh₃)₂]PF₆ (Noda *et al.*, 2006; Bag *et al.*, 1990). Recrystallization of the resulting green product by diffusion of diethyl ether vapour into a CH₂Cl₂ solution gave two forms of crystals, namely brown plates (minor component), (I), and green plates (major component), (II). We have already determined the structure of (II), which is an orthorhombic nonhydrated complex (Noda *et al.*, 2006). In this paper, we report the structure of (I), which is a monoclinic monohydrate, *trans*-[Ru^{III}(S₂COEt)₂(PPh₃)₂]PF₆·H₂O.



In compound (I), the structure of the cationic complex (Fig. 1) is very similar to that in (II), except for the orientation of the Et groups of the S₂COEt ligands. The Ru–P and Ru–S bond lengths, and the P–Ru–P bond angle (Table 1), compare well with those of (II) (Noda *et al.*, 2006).

The packing of (I) is illustrated in Fig. 2. There is positional disorder of the solvent water molecule. The P–Ru–P bond axis of the complex is aligned parallel to the [101] direction. This packing mode is different from that in the green orthorhombic crystal of (II).

Experimental

The preparation and analytical and spectroscopic characterization of the title Ru^{III} complex have been described previously by Noda *et al.* (2006).

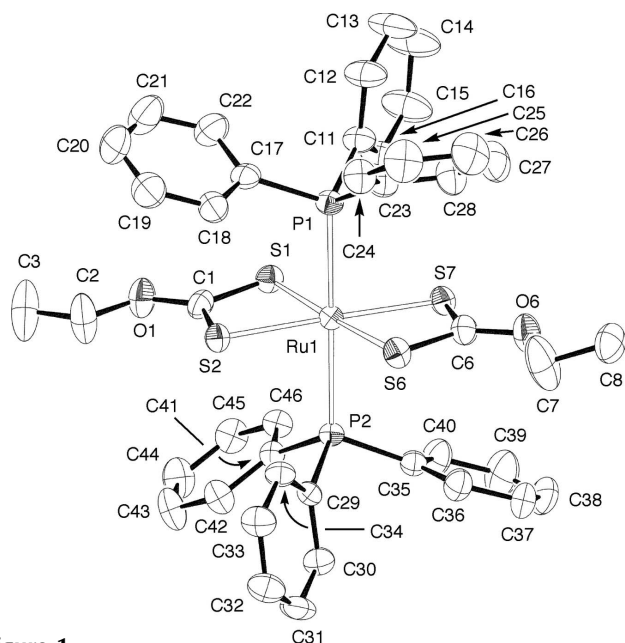


Figure 1
A plot of the cationic complex of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

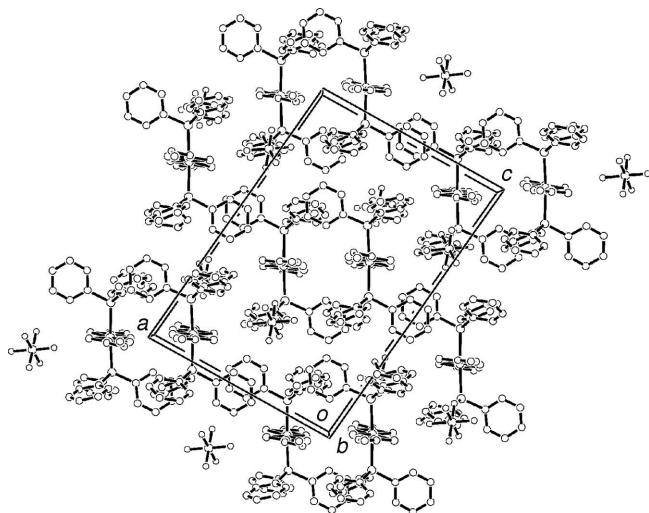


Figure 2
A packing diagram for (I). H atoms and the disordered water molecule have been omitted for clarity.

Crystal data

$[\text{Ru}(\text{C}_3\text{H}_5\text{OS}_2)_2(\text{C}_{18}\text{H}_{15}\text{P}_2)]\text{PF}_6 \cdot \text{H}_2\text{O}$	$V = 4626.5 (5) \text{ \AA}^3$
$M_r = 1030.98$	$Z = 4$
Monoclinic, $P2_1/n$	$D_x = 1.48 \text{ Mg m}^{-3}$
$a = 13.9877 (9) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 16.2122 (10) \text{ \AA}$	$\mu = 0.69 \text{ mm}^{-1}$
$c = 20.5103 (13) \text{ \AA}$	$T = 200 (2) \text{ K}$
$\beta = 95.904 (1)^\circ$	Platelet, brown
	$0.30 \times 0.22 \times 0.02 \text{ mm}$

Data collection

Rigaku/MSC Mercury CCD area-detector diffractometer	45552 measured reflections
ω scans	10523 independent reflections
Absorption correction: multi-scan (ABSCOR; Higashi, 1999)	8337 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.872$, $T_{\max} = 0.999$	$R_{\text{int}} = 0.045$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.058$
 $wR(F^2) = 0.156$
 $S = 1.12$
 10523 reflections
 541 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0619P)^2 + 6.0622P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.19 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Ru1—S1	2.3626 (11)	Ru1—S7	2.3618 (11)
Ru1—S2	2.3821 (11)	Ru1—P1	2.4497 (11)
Ru1—S6	2.3740 (11)	Ru1—P2	2.4426 (10)
S1—Ru1—S2	72.96 (4)	S2—Ru1—P2	83.82 (4)
S1—Ru1—S6	177.27 (4)	S6—Ru1—S7	73.10 (4)
S1—Ru1—S7	104.56 (4)	S6—Ru1—P1	92.58 (4)
S1—Ru1—P1	85.89 (4)	S6—Ru1—P2	85.22 (4)
S1—Ru1—P2	96.40 (4)	S7—Ru1—P1	87.52 (4)
S2—Ru1—S6	109.45 (4)	S7—Ru1—P2	93.91 (4)
S2—Ru1—S7	176.37 (4)	P1—Ru1—P2	176.90 (4)
S2—Ru1—P1	94.88 (4)		

H atoms bonded to C atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–0.99 \AA and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The solvent water molecule is disordered over two possible sites with occupancies of 50%. The water H atoms were located in difference syntheses and their positional parameters were fixed, with $U_{\text{iso}}(\text{H}) = 0.091 \text{ \AA}^2$ and O—H distances in the range 0.64–0.84 \AA . The volumes of the asymmetric units of (I) and (II) are 1156.6 (1) and 1107.5 (5) \AA^3 , respectively. A check with the program PLATON (Spek, 2003) revealed that the crystal structure of (I) contains solvent-accessible voids of 49 \AA^3 . However, no other solvent molecule was found in the difference map and the highest peak is located 0.93 \AA from atom O51.

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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