cis,cis-\(\mu\)-2,3,5,6-Tetra-2-pyridylpyrazine-\(\kappa^3N^1,N^2,N^6:\kappa^3N^3,N^4,N^5\)-bis-[dichloro(dimethyl sulfoxide-\(\kappa.S\))ruthenium(II)] dihydrate acetone disolvate

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Key indicators

Single-crystal X-ray study  
\( T = 120 \text{ K} \)

\( \text{Mean} \sigma(C{-}C) = 0.009 \text{ Å} \)

Some non-H atoms missing

\( R \) factor = 0.066

\( wR \) factor = 0.176

Data-to-parameter ratio = 21.3

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

The reaction of 2,3,5,6-tetra-2-pyridylpyrazine (tppz) with dichlorotetrakis(dimethyl sulfoxide)ruthenium(II) in dimethyl sulfoxide (DMSO) yielded the title centrosymmetric dinuclear complex, \( [\text{Ru}_2\text{Cl}_4(\text{C}_{24}\text{H}_{16}\text{N}_6)(\text{C}_3\text{H}_6\text{OS})_2]_2\text{C}_2\text{H}_6\text{OS} \cdot 2\text{H}_2\text{O} \) or \( \text{cis,cis-}[\text{Ru(DMSO)}\text{Cl}_2(\mu-\text{tppz})]_22\text{Me}_2\text{CO} \cdot 2\text{H}_2\text{O} \). Each ruthenium ion is in a distorted octahedral coordination in which the chloro ligands are cis to each other and DMSO is coordinated through sulfur. The asymmetric unit contains half of two independent molecules.

Comment

2,3,5,6-Tetra-2-pyridylpyrazine (tppz) has attracted a great deal of interest in supramolecular chemistry because it can function as a bis-tridentate bridging ligand (Fantacci et al., 2004). Crystal structures of dinuclear tppz complexes are mainly those of first-row transition metal ions (Carranza et al., 2003; Graf et al., 1997; Hadadzadeh et al., 2005; Campos-Fernandez et al., 2001). The only dinuclear RuII tppz crystal structure reported (Hartshorn et al., 1999) is that of \( \text{[Ru(Me}_2\text{bpy)}\text{Cl}_2(\mu-\text{tppz})]^{2+} \), where Me2bpy is 4,4'-dimethyl-2,2'-bipyridine.
growth occurred with the diffusion of acetone into the solution. Only the cis isomer was isolated and this is to be contrasted to the reaction of 2,2’-6’,2’-terpyridine (trppy) with Ru(DMSO)$_2$Cl$_2$, which gave both the cis and the trans-Ru(trppy)(DMSO)Cl$_2$ isomers, albeit in yields of 85 and 10%, respectively (Ziessel et al., 2004).

Crystallography revealed two acetone and two water molecules per complex molecule in the crystal structure. Two independent centrosymmetric complexes are found, with half of each in the asymmetric unit. The ruthenium ions display distorted octahedral coordination in which DMSO is sulfur-bound and the chloro ligands are in a cis geometry. Fig. 1 shows one of the two complexes, and it clearly shows the distortion from planarity of the tppz ligand in which two pyridyl groups coordinated to the same Ru$^{II}$ ion are tilted above the plane of the pyrazine ring, while the other two pyridyl groups coordinated to the second Ru$^{II}$ ion are tilted below the plane of the pyrazine ring. This conformation probably minimizes steric strain while at the same time maximizing the bonding interaction of the tppz ligand with the ruthenium ions. The shortness of the Ru—N(pyrazine) bonds (Table 1) is suggested to be due to the stronger π-accepting properties of the pyrazine ring.

**Experimental**

Ru(DMSO)$_2$Cl$_2$ (1 mmol) was dissolved in DMSO (20 ml). To the yellow solution was added tppz (0.5 mmol). The stirred reaction solution was heated to 333 K and the temperature maintained for two days, during which time the solution became deep purple in color. Addition of 600 ml of diethyl ether precipitated the purple product, which was collected and washed with diethyl ether. The crude product was recrystallized by diffusion of acetone into an aqueous solution of the complex. After four weeks, purple crystals formed. The yield was 90% based on tppz.

**Crystal data**

[ Ru$_2$Cl$_4$(C$_{14}$H$_{16}$N$_6$)(C$_2$H$_6$OS)$_2$2H$_2$O ]

$\gamma$ = 89.837 (7)$^\circ$

$V$ = 1925.3 (18) Å$^3$

$Z$ = 2

$D$$_{c}$ = 1.795 Mg m$^{-3}$

Mo $\text{Kx}$ radiation

$\mu$ = 1.22 mm$^{-1}$

$T$ = 120 (2) K

Plate, purple

0.18 × 0.15 × 0.04 mm

**Data collection**

Bruker APEX diffractometer

ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 2005)

$\tilde{\tau}$$_{\text{min}}$ = 0.751, $\tilde{\tau}$$_{\text{max}}$ = 0.953

8537 independent reflections

401 parameters

H-atom parameters constrained

**Refinement**

Refinement on $F^2$

$R$([$F^2$]) = 0.066

$wR$([$F^2$]) = 0.176

$S$ = 1.05

8537 reflections

$\chi^2$ = 2.46

401 parameters

**Table 1**

<table>
<thead>
<tr>
<th>Bond lengths (Å)</th>
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<tbody>
<tr>
<td>Ru1—N3 1.944 (5)</td>
</tr>
<tr>
<td>Ru1—N2 2.068 (5)</td>
</tr>
<tr>
<td>Ru1—N1 2.068 (5)</td>
</tr>
<tr>
<td>Ru1—S1 2.254 (18)</td>
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<tr>
<td>Ru1—Cl2 2.4112 (19)</td>
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<tr>
<td>Ru1—Cl1 2.4228 (18)</td>
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</table>

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**References**


metal-organic papers