

# Synthesis, characterization and antitumor properties of two highly cytotoxic ruthenium(III) complexes with bulky triazolopyrimidine ligands

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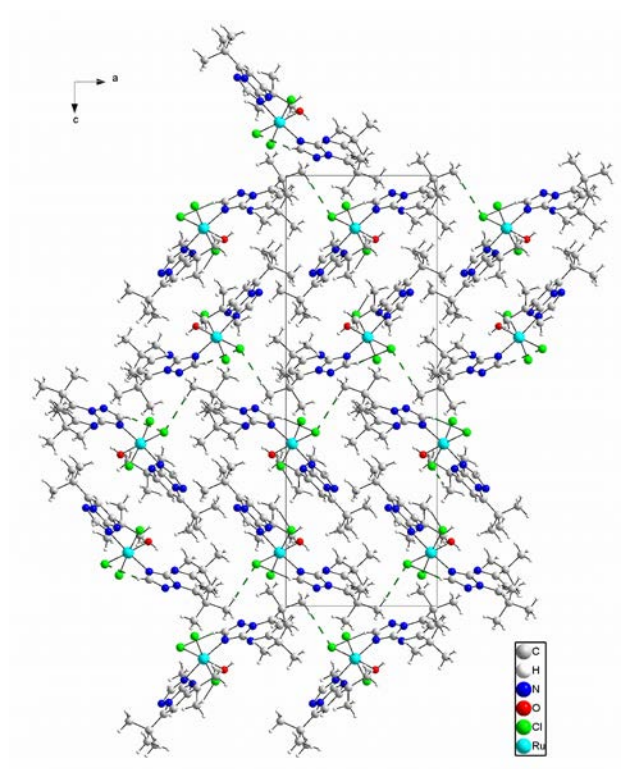
1. **Figure S1.** Packing of **1**.
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4. **Figure 4S.** Cyclic voltammograms of  $10^3$  M solutions of complex **1** in DMF (Fig. 4a) ( $E_p^{ox} = -0.36$  V and  $E_p^{red} = -0.29$  V), and complex **2** in DMF (Fig. 4b) ( $E_p^{ox} = -0.36$  V and  $E_p^{red} = -0.27$  V) with 0.1 M [nBu<sub>4</sub>N](PF<sub>6</sub>) at a scan rate of 0.1 V s<sup>-1</sup>.
5. **Table 1S.** Comparison of X-X distances and X-M-X angles in the studied octahedral ruthenium complexes containing halogen atoms and triazolopyrimidine as ligands.

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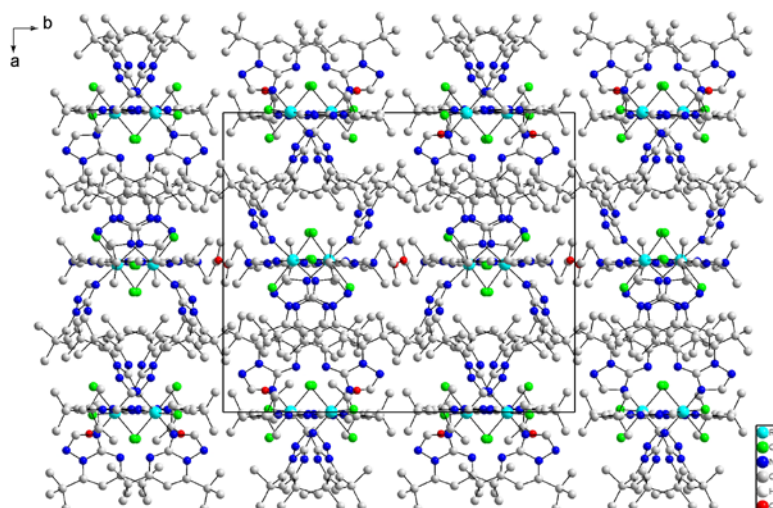
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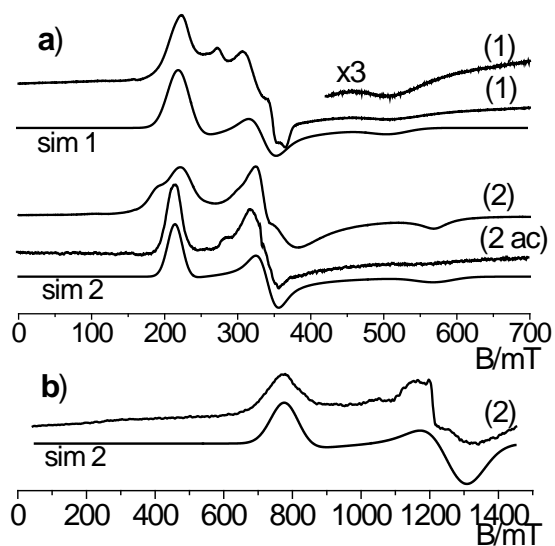
† Electronic supplementary information (ESI) available: CIF files and crystals packing of both ruthenium(III) compounds 1,2; CV and EPR spectra; comparison of X-X distances and X-M-X angles in the studied octahedral ruthenium complexes. CCDC 787821 1 and 901853 2. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c2dt32216a.



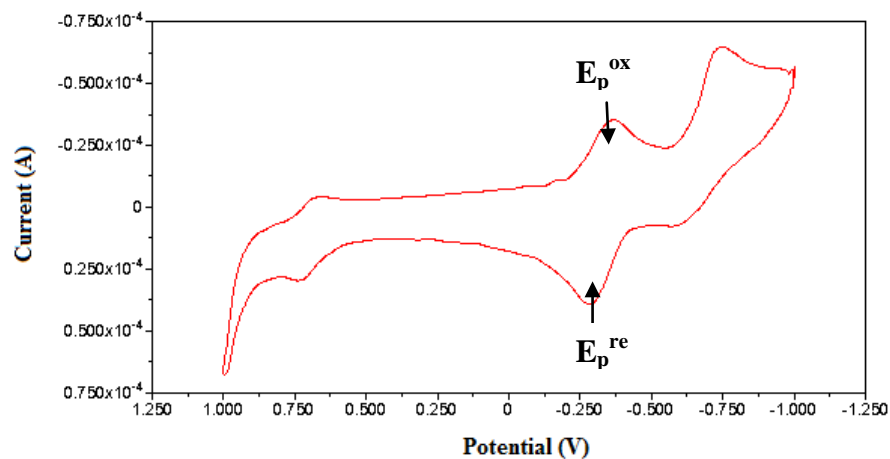
**Figure S1.** Packing of **1**.



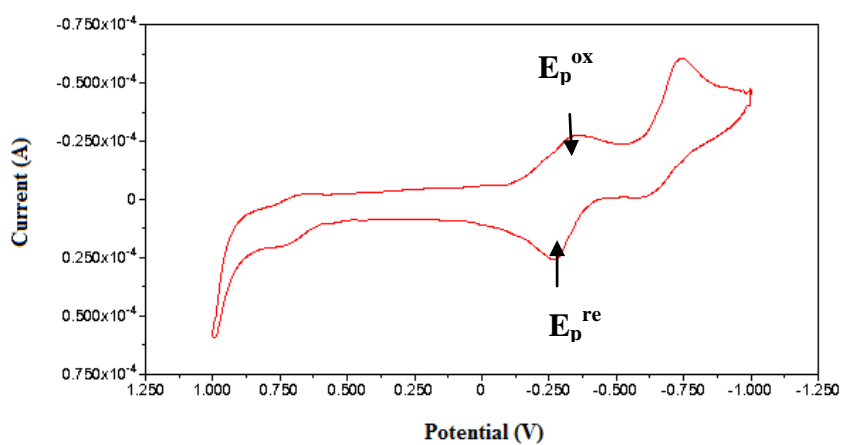
**Figure S2.** Packing of **2** with omitted hydrogen atoms and acetone molecule occurring only in one orientation (alternate structure was omitted for the clarity of the picture) along *c* axis reveals *bc* layers.



**Figure 3S.** The EPR spectra, (1) and (2), of powdered **1** and **2** complexes, respectively, and (2 ac) of the acetone solution of **2**, measured a) at X-band (9.581GHz) and b) at Q-band (33.98 GHz) and at 77 K, together with computer simulated spectra (sim **1** and sim **2**, respectively) using the spin Hamiltonian parameters given in the text.



**Fig. 4a**



**Fig. 4b**

**Figure 4S.** Cyclic voltammograms of  $10^{-3}$  M DMF solutions of complex **1** (**Fig. 3a**) ( $E_p^{ox} = -0.36$  V and  $E_p^{red} = -0.29$  V), and complex **2** (**Fig. 3b**) ( $E_p^{ox} = -0.36$  V and  $E_p^{red} = -0.27$  V) in 0.1 M  $[nBu_4N](PF_6)$  at a scan rate of  $0.1 \text{ Vs}^{-1}$ .

**Table 1S.** Comparison of X-X distance and X-M-X angle in selected octahedral ruthenium complexes with halogen atoms and triazolopyrimidine as ligands.

Compound	M-N [Å]	M-X [Å]	X-X [Å]	X-M-X [°]	REF.
<i>trans</i> -[RuCl <sub>3</sub> (H <sub>2</sub> O)(dbtp) <sub>2</sub> ]	2.074	and 2.3118,	3.323,	91.74,	This paper
	2.075	2.3182,	3.348,	92.33	
		2.3291	4.644	175.36	
<i>mer</i> -[RuCl <sub>3</sub> (dbtp) <sub>3</sub> ].0.829OCMe <sub>2</sub>	2.050,	2.350,	3.340,	89.97,	This paper
	2.067,	2.3520,	3.342,	90.00,	
	2.076,	2.3551,	3.375,	91.10,	
	2.085,	2.363,	3.390,	91.98,	
	2.093,	2.364,	4.707,	177.99,	
	2.094	2.3723	4.713	178.52,	
<i>trans</i> -[RuCl <sub>3</sub> (dmtp) <sub>2</sub> (9-methyladenine)].½CH <sub>2</sub> Cl <sub>2</sub>	2.035 (adn)	2.333,	3.364,	89.89,	9
	2.090	and 2.377,	3.366,	91.03,	
	2.083	2.385	4.710,	178.64	
<i>trans</i> -[RuCl <sub>3</sub> (H <sub>2</sub> O)(dmtp) <sub>2</sub> ]	2.092(4)	2.306(2)	3.331	91.8(1)	5a
	2.092(4)	2.331(2)	3.342	90.1(1)	
	2.101(4)	2.388(2)	4.693	178.0(2)	
	(Ru1-O1)*				
<i>mer</i> -[RuCl <sub>3</sub> (H <sub>2</sub> O)(dmsO)(dmtp)].H <sub>2</sub> O	2.137(2)	2.313(1)	3.360	94.22	4
	2.267(1)	2.332(1)	3.407	92.66	
	(Ru1-S1)	2.337(1)	4.659	172.77	
	2.094(2)				
(Hdmtp) <i>trans</i> -[RuCl <sub>4</sub> (dmsO)(dmtp)].¼Et <sub>2</sub> O	(Ru1-O2)				4
	2.121(8)	2.329(2)	3.442	94.73	
	2.255(2)	2.346(3)	3.262	87.62	
	(Ru1-S1)	2.349(2)	3.295	89.62	
		2.364(3)	3.273	88.04	
			4.691	175.22	
		4.692	177.63		