Poster

Crystal structures of rhenium(V) complexes with thiosemicarbazonate ligands

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The radionuclide technetium-99m, thanks to its ideal physicochemical properties and availability, is the most used radionuclide in clinical practice, for the SPECT imaging (Single Photon Emission Computed Tomography), the first-line imaging modality in nuclear medicine. Recently, the radionuclide ^{188}Re emerged as a very attractive candidate for endoradiotherapy due to its nuclear features.[1] Since many studies demonstrate the biodistributive equivalence of stable technetium and rhenium complexes with same coordination spheres, the parallel study of the coordination chemistry of these elements is crucial to develop a *matching theranostic pair* that combines diagnosis and therapy [1, 2]. Here, we describe crystal structures obtained in a coordination chemistry study of $[ReN]^{2+}$ and $[ReO]^{3+}$ cores with thiosemicarbazones (TSCs), an interesting class of ligands very little explored in conjunction with these cores up to now [3,4]. The TSCs considered in this study are 3-methoxysalicylaldehydethiosemicarbazone (H_2L1) and N,N-dimethyl-3-methoxysalicylaldehydethiosemicarbazone (H_2L2).

Crystals of the ligand precursor H_2L2 show tabular, green habitus and belong to space group $P2_1/n$. The molecule shape and the bond lengths indicate significant electron delocalization. The thioureic bond is in *Z* configuration, which is unusual for this class of molecules, and it is very likely due to intramolecular interactions different from typical ones for TSCs [5]. Crystals of nitrido-complexes $[ReN(L1)(PPh_3)]$ (fig. 1a) and $[ReN(L2)(PPh_3)]$ show prismatic, red and tabular, orange habits and belongs to space groups $P2_1/n$ and $P\bar{1}$, respectively. The complex coordination polyhedra are square-base pyramid, with nitrido ion in apical position. Crystals of oxo- complex $[ReO(L2)(HL2)]$ (fig. 1b) show tabular, red habit, and belong to space group $P2_1/c$. The coordination geometry is octahedral: a tridentate thiosemicarbazonate-phenolate is bounded in *fac* coordination mode with oxygen donor atom in *trans* with respect to oxydo ion, and a bidentate thiosemicarbazonate is coordinated at equatorial position. In all complexes, the bond lengths indicate a decrease of electronic delocalization in respect to the non-coordinated proligand.

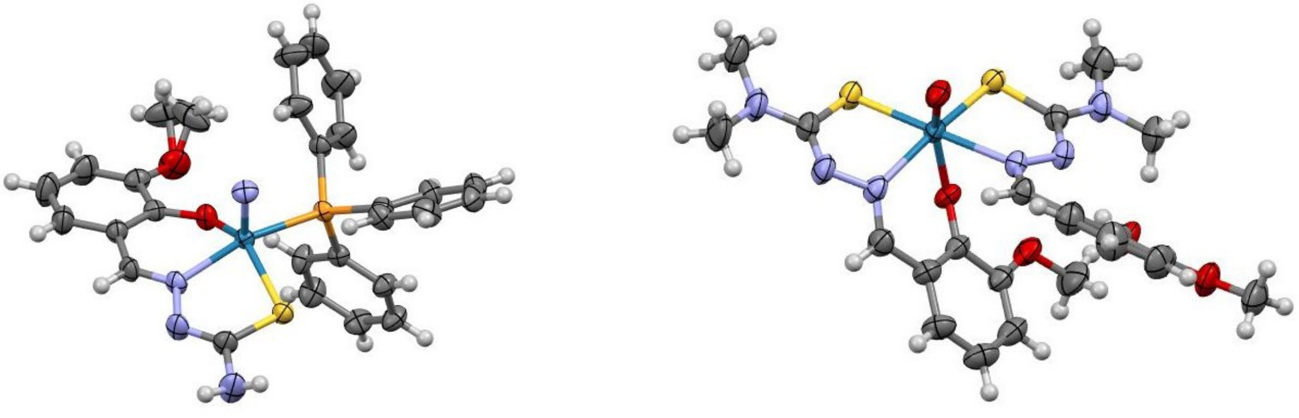

Figure 1. ORTEP diagram of complex a) $[ReN(L1)(PPh_3)]$ and b) $[ReO(L2)(HL2)]$. Colour code: turquoise-rhenium, grey-carbon, white-hydrogen, blue-nitrogen, red-oxygen, yellow-sulfur, orange-phosphorous.

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