

Synthesis, Structure and Properties of Two Symmetrical Oxorhenium(V) Dimers Derived From 4-Chloro Pyrazole

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Oxorhenium(V) complexes are of considerable interest due to their multifaceted applications in the field of catalysis and in radiopharmaceuticals. The properties of these oxo-complexes can be “fine-tuned” through appropriate ligand choices. Our lab has been engaged in the development of coordination chemistry with pyrazoles due to their versatile binding modes. Pyrazole can bind a metal center in either monodentate or bridging bidentate fashion. Moreover, the 3, 4, and 5-positions on pyrazole ring offer the opportunity for suitable functionalization for desired applications. Although there has been a plethora of research work on transition metal coordination complexes involving pyrazole(s), there is a paucity of analogous oxorhenium(V) systems. This has prompted us to explore the possibility of isolating oxorhenium(V) complexes with pyrazole(s). In that endeavor we have successfully synthesized two oxorhenium(V) dimeric systems, namely, $[\text{ReO}_2(\text{m-4-Clpz})_2\text{Cl}_2(\text{PPh}_3)_2]$ (**1**) and $[\text{ReO}_2(\text{m-O})(\text{m-4-Clpz})_2\text{I}_2(\text{PPh}_3)_2]$ (**2**) through the reactions of $[\text{ReO}(\text{OEt})\text{Cl}_2(\text{PPh}_3)_2]$ and $[\text{ReO}(\text{OEt})\text{I}_2(\text{PPh}_3)_2]$ respectively with 4-Cl-pyrazole in 1:2 molar ratio. The molecular structure of complex **2** has been authenticated by single crystal X-ray crystallography. X-ray structure revealed the dimeric structure of complex **2**, where each Re center resides in a distorted octahedral coordination environment. The two 4-Cl pyrazolato ligands binds the two metal centers as bridging bidentate fashion. In the structure there are two terminal oxo groups, for which the Re-O bond lengths suggested double bonded character. There is also a μ_2 -bridging O^{2-} located in this dimeric structure. The two complexes are also characterized with other conventional analytical techniques.