

Exploiting existing rhenium piano-stool complexes as synthon for facile library generation and potential medicinal applications

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In this master thesis, two different approaches were investigated for synthesizing rhenium piano-stool complexes bearing a diimine and a halide ligand. The first one involves a Fischer-Hafner synthesis applied to rhenium oxo-complexes. The second one focuses on ring abstraction of a rhenium sandwich complex. The halide ligand is labile and can be easily exchanged. The resulting complex would be a versatile synthon for further synthetic purposes. The acetonitrile ligand in already existing complexes, such as $[\text{Re}(\eta^6\text{-C}_6\text{H}_6)(\text{N}^{\wedge}\text{N})(\text{NCCH}_3)]^+$, was found to be more labile than initially expected, making these complexes effective synthons.

A library of different complexes where acetonitrile is replaced by other nitrogen-based ligands was generated and characterized by NMR, UV-Vis, IR, and ESI-MS. The stability of $[\text{Re}(\eta^6\text{-C}_6\text{H}_6)(\text{bipy})(\text{py})]^+$, the simplest member of this library, was investigated in various solvents, along with its behavior under light exposure at different wavelengths. Computed UV-Vis, experimental UV-Vis measurements and orbitals involved in these transitions were compared to elucidate some stability observations. This study could open the possibility of developing a new branch in photoactivated chemotherapy (PCT), with benzene-releasing molecules.

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