Synthesis and Characterization of Homo- and Heteroleptic Niobium(V) Complexes. Exploration of Their Catalytic and Biochemical Potential

A thesis submitted in partial fulfilment of the requirements

for the degree of

DOCTOR OF PHILOSOPHY

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August, 2023

Conclusions and Future Scope

Conclusions

In this thesis, we have reported series of simple, sustainable, and highly efficient heterogeneous and homogeneous catalyst systems by anchoring peroxidoniobium(V) species to insoluble as well as water-soluble synthetic or natural polymer support, including appropriately functionalized cross-linked PS-DVB resin, biopolymer chitosan and water-soluble poly(sodium methacrylate). The developed catalysts represent promising avenues in the oxidative transformations of a range of organic substrates, *viz.*, oxidation of sulfides to sulfoxides/sulfones, epoxidation of olefins, oxidation of 5-hydroxymethyl-2-furfural to 5-hydroxymethyl-2-furancarboxylic acid and hydroxylation of phenol to dihydroxybenzene with outstanding yield, TON along with high product selectivity. All of these oxidation processes were carried out in the presence of the green oxidant H_2O_2 under ecologically compatible mild reaction conditions. Safety, utilization of bio-inert and non-toxic metal (Nb) as well as environment-friendly starting material for catalysts preparation, easy handling, regeneration, and reusability of the catalysts with undiminishing activity/selectivity profile are some of the significant features of these catalytic protocols. Moreover, the unique properties of the developed triperoxidoniobium(V) derivatives, such as their versatility, robustness, high reactivity under aqueous medium, and selectivity, make them attractive candidates as water-compatible and water-tolerant catalysts for a variety of catalytic applications.

Furthermore, the potential application of the water-soluble macromolecular as well as monomeric triperoxidoniobium(V) compounds and the tris(maltolato)oxidoniobium(V) complex as enzyme inhibitors opens up new prospects for the designing of therapeutics targeting different diseases and pharmaceutical research. The preparation, characterization and kinetics inhibition studies of these compounds towards the enzyme acid phosphatase have furnished valuable insights into their structure-activity relationships as well as mechanisms of action.

Future Scope

Moving a step towards the development of various niobium(V) based catalysts as well as enzyme inhibitors unveils several exciting research directions. For our future work, we have a few proposed projects in different directions where we can directly implement the results of this thesis work.

By varying the co-ligand environment with other polymers as well as auxiliary ligands possessing varied physicochemical and bio-relevant properties and further investigation of their catalytic abilities could afford more efficient and selective Nb-based catalysts for industrially important organic oxidative transformations. This could have substantial contributions to the fine chemical, pharmaceutical, and agrochemical industries.

Persistent endeavors to elucidate the structural factors influencing the interaction of niobium(V) based complexes with various enzymes may facilitate the rational designing of novel enzyme inhibitors exhibiting greater potency and specificity. In addition to that, exploration of the biocompatibility and pharmacokinetic properties of such Nb(V) compounds will be vital for their implementation in clinical approach. Methodologies for achieving targeted delivery and regulated release of those compounds could augment their therapeutic value by minimalizing the adverse effects.

Through interdisciplinary approaches integrating chemical, biological, as well as computational modeling, we can extend our study of niobium in such a manner that it could improve our understanding of the various niobium(V) catalysts and enzyme inhibitors and thus, develop greener chemical processes and new drugs. Such extended and extensive research may hold the greater ability to address the challenges in catalysis and drug discovery, thereby paving the way to both scientific knowledge and societal well-being.