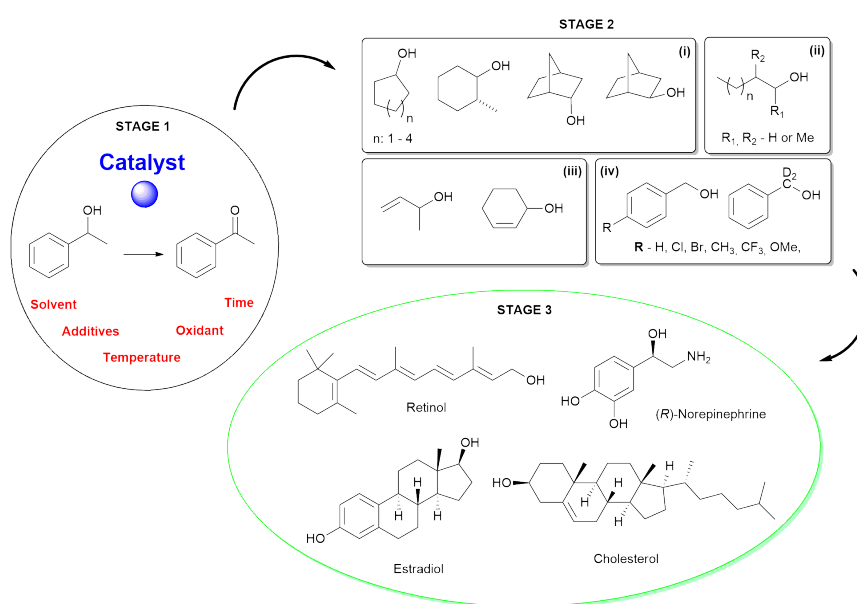


Research project objectives

Scientific goal of the project “New libraries of Schiff-base complexes as a way for rational design of alcohol oxidation catalysts” involves the synthesis, spectroscopic and structural characterization of new transition metal complexes aimed at investigation of their catalytic properties. One of the main challenges in catalysis is to pursue a correlation between structure/specific properties and such can be achieved by synthesis of small libraries of constitutionally similar ligands. Their complexation and further screening in terms of catalytic properties allows one to gain further knowledge on the factors, that render efficient i.e. fast and selective organic transformations possible, herein alcohol oxidation. Furthermore, our catalysts are anticipated to become an alternative to commonly used toxic and environmentally hazardous oxidants.

Basic research

Realization of the former projects was an inspiration to design new coordinating agents with one/two tridentate chelating coordination pocket(s) constituted on imidazole scaffoldings. Ten new, easily accessible Schiff base ligands were designed, so as to encompass N-heterocyclic moieties (pyridine, imidazole, benzimidazole) and thus form one or two preorganized tridentate meridional binding units that account coordinative preferences of d-block elements to nitrogen donor atoms. The latter ones are anticipated to self-assemble into simple (mononuclear) and/or sophisticated (grids, clusters, polymers) metallo-supramolecular architectures, which are further going to be studied for their catalytic properties. Particular attention shall be given to the emergence of such systems, that display notable catalytic behavior, i.e. are efficient in terms of oxidation of primary and secondary alcohols.



Those in turn are going to be rationalized in terms of structure/property dependencies, thus emphasizing appropriate design of new coordinating agents.

Research project impact

Polypyridine supramolecular architectures represent a fascinating class of compounds due to structural diversity they expose and consequently giving access to plethora of potential applications, those include supramolecular engineering, nanotechnology, biomedical inorganic chemistry, biological catalysis and materials chemistry. Individual physicochemical properties of incorporated metal ions are responsible for behaviour of synthesized complexes, therefore such that may adopt different oxidation states and exhibit stereochemical nonrigidity are of particular interest. Aforesaid combination of traits, makes transition metal ions an ideal metallic centres for research, particularly in the field of catalysis.

Selectivity and activity are two most important parameters that characterize desired catalysts. Rationalization of ligands structure appears to be the key factor in order to enhance those, nonetheless it is hard to present general rules or prerequisites for efficient systems. In fact, some prominent chemical processes have indeed been found by serendipity rather than through rational thought processes. As a result, various metal centres – iron in particular – are subjected to miscellaneous N-heterocyclic ligands to form active catalysts, utilized in different organic transformations.

We believe presented project will significantly contribute to the knowledge expansion of self-assembly driven formation of various metallosupramolecular architectures, but at the same time it will highlight the importance of appropriate design of new coordinating agents, which will result in synthesis of new libraries of efficient alcohol oxidation catalysts.