Project 3.5 Activation of Dinitrogen by Multinuclear Iron and Vanadium Complexes Supported by Sterically Demanding N, N-ligands

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Background:

A persistent challenge in chemistry is to activate and functionalize atmospheric N2 molecules. The utilization of this abundant molecule for the synthesis of N-containing valuable products typically requires a prior activation of an N2 molecule at a redox-active metal center. In biological nitrogen fixation, Nature uses metalloenzyme systems called nitrogenases, among which the most efficient contains a multinuclear molybdenum-iron cofactor, but systems involving iron–vanadium and iron-only cofactors are also known. These chemical transformations by nitrogenases represent biological equivalents to the industrial, where heterogeneous iron or ruthenium catalysts are used in order to convert N2 and H2 to NH3. Hence, both the coordination chemistry of N2 species and the search for processes that involve a homogeneous catalyst for the utilization of N2 as a feedstock to generate higher-value organonitrogen materials are continually one of the greatest challenges facing chemists. The proposed project is focused on designing new reaction systems based on multinuclear low-valent iron complexes tailored with ligands featuring two monoanionic N, N-binding sites for fundamental studies of the N2 activation and transformations.

Aim:

The project aims to design, synthesis, and structural characterization of new iron and vanadium complexes supported by ligands featuring monoanionic N, N-binding sites. Next, the developed coordination systems will be utilized for the N2 activation and reduction in the presence of various reducing agents. Modification of the N, N-binding sites will affect the nuclearity of molecular systems and spatial distribution of metal centers, which will shed new light on the cooperativity and synergic effects of multiple metal centers in the N2 activation processes.

Requirements:

- MSc degree in chemisty, physics, or related science fields,
- fluency in English in writing and speech,
- basic experience in inorganic synthetic methods and characterization of materials (e.g. NMR, PXRD, IR, MS, UV-Vis)