Project 3.13 Oxygenation processes of organometallics with non-redox active metal centers

Supervisor: Prof. Janusz Lewiński, PhD Dsc. Eng. / Adam Kubas, PhD Dsc.
Institute: Physical Chemistry PAS
Research group: Research group No. 9. Coordination metal complexes and functional materials – prof. dr hab. inż. Janusz Lewiński
www: http://lewin.ch.pw.edu.pl/

Background:

A persistent challenge in chemistry is to activate of dioxygen molecules in the controlled manner. The utilization of this abundant molecule for oxidation reactions typically requires a prior activation of a O2 molecule at a metal center. Mechanistic studies on the O2 activation by redox-active transition metal complexes have provided various activation pathways and strategies for circumventing unwanted radical reactions.

Hence, for decades, mechanistic research has been dominated by the reactions of O2 with transition metal complexes. In turn, this is not the case of the oxygenation reactions involving organometallics with non-redox-active metal centers. Notably, reactions between O2 and organometallics with non-redox-active metal centers have received continuous interest for over 160 years, however significant uncertainties concerning the character and details of the actual mechanism of these reactions persist to the present days, including the initiation process and further transformations of the formed reactive oxygen species. Our research group is continuously envisioning unforeseen breakthroughs in the oxygenation of organometallics with non-redox centers, i.e., one of the oldest problem in the organometallic chemistry, on the level of mechanistic considerations and potential applications.

Aim:

The proposed project aims to further advancing the fundamental knowledge of the oxygenation processes and factors controlling the character and reactivity of the resulting products. Specific objectives include: i) design, synthesis and characterization of new model organometallic complexes (M = Mg, Zn, Al, Ga, In) of an appropriate coordination sphere environment around the metal center supported by various multidentate ligands, ii) reactivity studies of the resulting organometallics towards O2 in order to elucidate critical factors in the oxygenation of metal alkyls with redox-inactive centers (like the character of metal center, metal bonded alkyl substituents and supporting ligands and the role of noncovalent interactions on the reaction courses), iii) development of new synthesis routes of metal alkoxides and alkylperoxides, iv) elucidation of the intimate steps in the oxygenation of metal alkyls via theoretical studies.

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);
- basic knowledge of computational and simulation techniques.