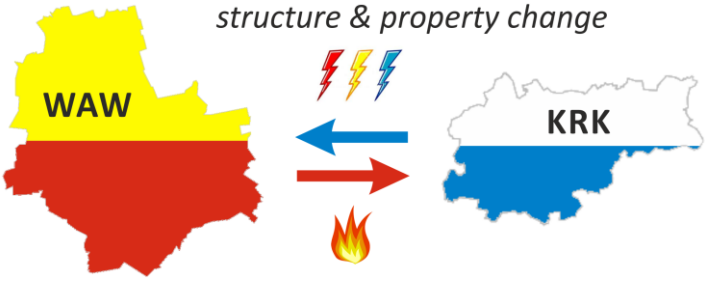
MXO2-ISOMER: in search of colour-changing photoswitchable materials based on 4th-row transition-metal complexes with simple ambidentate ligands



Colour-changing photoswitchable materials (idea illustrated humorously on the example of two Polish cities – Warsaw and Cracow).

Interaction of light with matter is one of the key processes occurring in nature. Deep understating of its character and associated phenomena is crucial for conscious design of novel functional materials with desired properties. Therefore, chemical compounds exhibiting specific photoactive properties, either in solution or, even more importantly, in the solid state, are among the most desired materials nowadays. Photoactive materials may find various applications in the fields of optoelectronics or medicine, as well as, in solar energy conversion and data storage technologies. In view of the above, photoswitchable compounds are particularly interesting. Their structure can be modified via external stimuli (light, temperature), which influences the change in their micro- and macroscopic properties. One can easily imagine novel materials based on photoswitchable chemical systems, which can be applied, for example, as various colour-changing coatings (e.g. car body, contact lenses, etc.) controllable via external perturbation. This idea constituted the inspiration for the current research project.

Consequently, the proposed project is dedicated to thorough and systematic investigations of the light-induced processes occurring in crystals of selected Fe, Ni and Co complexes containing ambidentate nitro and/or sulphur dioxide ligands. Such ligands can switch from one binding mode to another upon light irradiation or temperature changes. In turn, the choice of metals is dictated by their availability, price, and, most importantly, the relatively easy modification of their complexes facilitated by exchanging various ligands, therefore allowing for considerable structural diversity, molecular flexibility, different molecular environment in a crystal, and also various numbers of photo-switchable fragments bound to a metal centre. Such selection will enable studies of various factors' effects on the nitro and sulphur dioxide linkage isomerisation, allowing comparison between different metal centres, ligands, intermolecular interactions, charges on metal atoms, etc. In addition, we intend to rate the influence of temperature on the transformation under investigation, the reversibility of the analysed process and the stability of the created linkage isomers. We shall start our investigations with model nitro and sulphur dioxide Fe, Ni and Co coordination compounds, selected based on our experience in this matter and literature reports, whereas then we shall apply modifications to these systems. We plan to investigate such compounds and their properties starting from the synthesis, through crystallisation, spectroscopic, structural and other physicochemical analyses, to photocrystallographic methods. The experimental results will be supplemented by theoretical modelling, in order to propose a possible mechanism of the reaction in the solid state and rate the mutual stabilities of different binding modes of NO_2 and SO_2 moieties.

We believe that the obtained results will provide us with effective colour-changing photoswitchable compounds and/or information on the modifications needed to obtain promising functional materials, characterised by desired spectroscopic properties, reversibility, high conversion percentage and stability, appropriate for further technological applications.