RUHR-UNIVERSITÄT BOCHUM

RUB

SPECIALIZATION / MASTER / PHD PROJECT AVAILABLE!

Photochemical reactions of chiral molecules in cryogenic matrices

The overarching project: Vibrational circular dichroism (VCD) spectroscopy is the chiral version of IR spectroscopy. It allows us to gain information on absolute configurations and intermolecular interactions of chiral molecules. Often these insights are more detailed than what can be achieved by NMR spectroscopy or IR alone. We have combined VCD spectroscopy with the matrix isolation (MI) technique that allows the characterization of reactive intermediates that are generated for instance photochemically or by pyrolysis. MI involved the isolation of suitable precursors in cryogenic solid matrices, e.g. of argon or neon at 25K and 4K, respectively. MI-VCD spectroscopy has been shown to be a great tool to characterize the vibrational spectra of small chiral molecules, and very recently we have demonstrated for the first time that also chiral photochemically generated species can be characterized (*ACIE* **56** (2017) 1925).

Topic for the thesis (and beyond?): In this project, we want to further explore the possibilities of MI-VCD and focus on chiral ring opening reactions that proceed from a chiral precursor via a chiral intermediate conformation to achiral products. We want to use MI-VCD to capture this intermediate conformation in order to learn about torque selectivities of reactions. Furthermore, we want to prepare chiral radicals and carbenes and characterize their structures using MI-VCD. These experiments will be particularly interesting to challenge the current state-of-the-art theory of VCD. Lastly, we want to go beyond classical matrices of Ar or Ne and use para-hydrogen (pH_2) as host environment. This requires the construction of a pH2 generator and the rigorous testing of both the generator and the pH2-matrix instrument. For the aforementioned studies, pH2 can be a very interesting environment as energy dissipation for instance arising from the thermal relaxation of photochemically excited states is fast. Solid pH2 also possess "self-healing" capabilities, i.e. the crystal lattice quickly relaxes after a photochemical reaction changes the volume of the encapsulating matrix site.

Who are we looking for? That depends on the part of the project you want to work on!

- Someone with interest in physical organic chemistry and spectroscopy
- For work on photochemical reactions, you ideally have some interest and experience in organic synthesis in order to be able to make your precursors.
- pH2 matrices: A tinkerer and spectroscopist, who is very precise and accurate, as the development of a new spectroscopic technique is challenging on its own!

For more information contact Prof. Dr. Christian Merten directly.

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