

12th June 2014 - 10:00
 Building 99, Seminar Room I and II (EG)

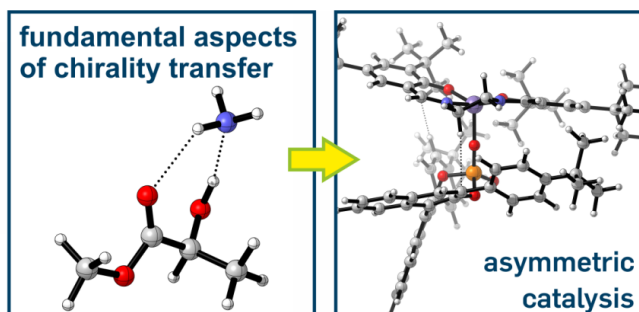
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**Probing intermolecular interactions using VCD spectroscopy:
 From noble gas matrices to asymmetric catalysis**

Vibrational Circular Dichroism (VCD) spectroscopy measures the small difference in the absorption of left- and right circular polarized infrared light by a chiral sample. It allows the unambiguous assignment of absolute configurations by comparison of experimental VCD spectra with computationally predicted spectra. Besides its unique sensitivity to chirality and absolute configurations, VCD spectroscopy is highly sensitive to even very subtle differences in structures, such as conformational changes induced by solute-solvent interactions.

In our work, we take advantage of this conformational sensitivity and use VCD spectroscopy to probe intermolecular interactions in solution and in solid noble gas matrices under matrix-isolation (MI) conditions. We are particularly interested in understanding mechanisms of chirality transfer in catalysis. Thus, we study the intermolecular interactions between chiral and achiral molecules which can be mediated through different kinds of interactions (Coulomb interactions, hydrogen and dihydrogen bonding, halogen bonding etc.) and which cause a locking of the achiral molecule in a chiral conformation. At a more fundamental level, we are interested in implementing new sampling techniques for VCD spectroscopy, such as the matrix-isolation (MI) technique. MI-VCD studies allow us to get a much closer insight into the conformational preferences of chiral molecules and their intermolecular interactions.



In this talk, I will give a brief introduction to the spectroscopic technique, followed by a discussion of various examples spanning from chiral transition metal complexes^[1] and organocatalysis^[2] in solution to fundamental spectroscopic and theoretical aspects regarding anharmonic effects in vibrational spectra^[3] or misleading vibrational band assignments.^[4]

[1] C. Merten, R. McDonald, Y. Xu, *Inorg. Chem.*, **43**(2014) 3177-3182

[2] C. Merten, S. Liao, B. List, *under preparation*

[3] C. Merten, J. Bloino, V. Barone, Y. Xu, *J. Phys. Chem. Lett.* **4** (2013) 3424-3428

[4] C. Merten, Y. Xu, *ChemPhysChem*, **14** (2013) 213-219