RUHR-UNIVERSITÄT BOCHUM

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SPECIALIZATION / MASTER / PHD PROJECT AVAILABLE!

Implementation of a new setup to record IR spectra in liquid rare gases and its application in the determination of thermodynamic parameters of weakly bound clusters

Background: Non-covalent interactions play an important role in steering chemical reactivity in general as well as in controlling superstructure formation in supramolecular chemistry and biochemistry. While hydrogen bonding interactions are well understood, halogen bonding interactions are currently emerging as new design element for many applications. Therefore, being able to computationally predict interaction energy would be of great advantage. When interested in neutral donors and acceptors, however, experiment and theory are not entirely compatible yet: The most accurate computational models require so small model systems (e.g. $F_3C\text{-}I\bullet\bullet N(CH_3)_3$) that experimental data on binding enthalpies, for instance, is hard to obtain with conventional thermochemical methods.

The overarching project: We have recently developed a setup that allows us to record IR spectra with liquid rare gases (LRg) as solvent. LRg have the advantage of being completely inert and not interfering with the formation of weakly bound clusters. In addition, liquefying rare gases requires elevated pressures (5-10 bar) and low temperatures (-100°C). Hence, when the Rg is mixed with interaction partners in gas phase, they are dissolved in the LRg after condensation of the mixture and can then be investigated. This includes the aforementioned example of $F_3C\text{-}I\bullet\bullet N(CH_3)_3$! The experiments allow us to extract binding enthalpies by temperature dependent measurements with an experimental accuracy of < 0.5 kcal/mol. Finally, these experimental numbers allow us a critical comparison with computed data and thus guide the development of computational protocols.

Topic for the thesis (and beyond?): In this thesis project, you will build a second setup for LRg measurements analogously to the existing one. The difference is that the new setup will have an IR cell with 5 cm path length (as opposed to the existing system with 7 mm), which is suited for experiments with liquid argon. You will benchmark the system using a known and well characterized halogen bonding model system and continue determining binding enthalpies for further systems. Your experiments will be complemented by computational spectra predictions.

Who are we looking for?

- Someone with interest in physical (organic) chemistry and spectroscopy
- A tinkerer with interest not only in doing experiment, but in building them

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

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