

Module time: 5-6 hours

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Contact: ginny.karir@ruhr-uni-bochum.de, dirk.grote@ruhr-uni-bochum.de, wolfram.sander@ruhr-uni-bochum.de

Understanding Microsolvation using Matrix Isolation FTIR Spectroscopy and *Ab Initio* Calculations- A Window to Non-Covalent Interactions

Theory : Microsolvation of the solute molecules in a solvent generally involves an interplay of many non-covalent interactions. One such example of non-covalent interaction is hydrogen bonding which is known to influence the structure and hence reactivity of solute molecules. Vibrational spectroscopy is a powerful spectroscopic tool to study hydrogen bonding interactions. However weak to very weak hydrogen bonding interactions such as $\text{O-H}\cdots\pi$ and $\text{C-H}\cdots\text{O}$ are difficult to observe experimentally in condensed phase due to spectral broadening. This spectral broadening is caused by the presence of intermolecular interactions between the solute molecules in bulk media and doppler broadening at room temperature and masks the vibrational features of hydrogen bonded solute-solvent complexes. In matrix isolation FTIR spectroscopy (Fig 1), solute molecules are diluted with large excess of inert gas (1:1000) such as Ar, Xe, N_2 and the resulting mixture is deposited on a cold substrate (Csl) kept at 3-10 K under the vacuum of 10^{-6} mbar. This solidified film can then be probed by FTIR spectroscopy. The technique results in a spectrum with very sharp vibrational features and hence can be used to probe the non-covalent interactions responsible for microsolvation.

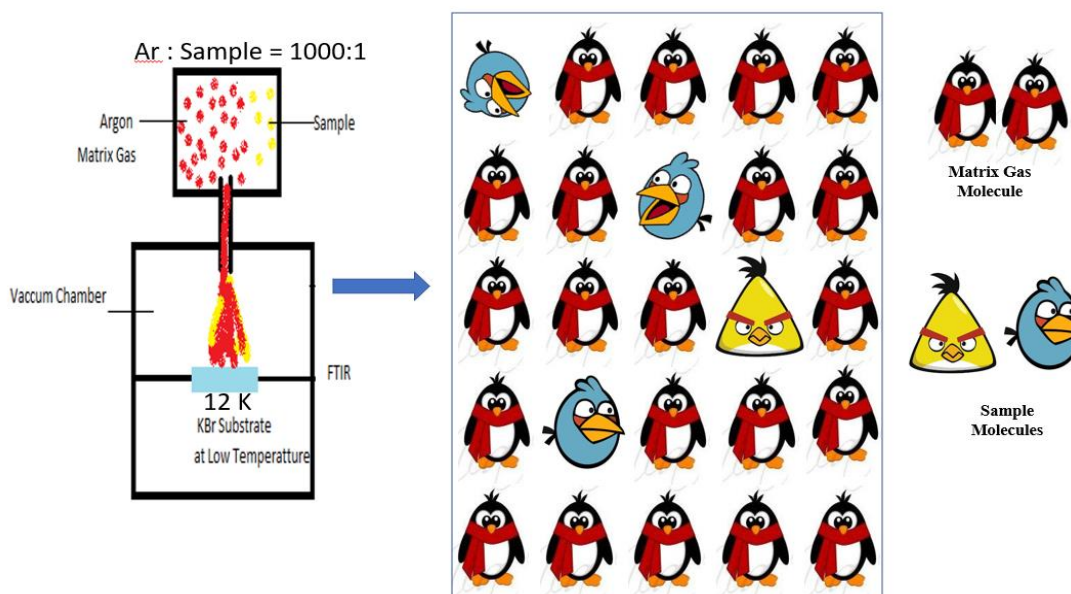


Fig 1. Matrix Isolation FTIR Spectroscopy.

In this module students will learn about the technique of matrix isolation FTIR spectroscopy and its use in probing weak non-covalent interactions such as hydrogen bonding. This includes practical demonstration of the experimental procedure, sample preparation, data acquisition and data analysis.

1. Recording liquid phase and matrix isolated FTIR spectra of solute and solvent molecules and their comparison in terms of FWHM of the vibrational features.
2. Identifying solute-solvent hydrogen bonded dimers experimentally.
3. *Ab Initio* computations of hydrogen bonded complexes between phenylacetylene (solute) and water (solvent) and subsequent computation of interaction energies of optimized complexes, vibrational frequencies and isotopic shifts.
4. Corroborating experimental and computational data.