AG: Sander

Autor/Betreuer: Dirk Grote

Matrix Isolation and EPR spectroscopy of Solvent Complexes

Matrix Isolation can be used as a tool to study weak interactions between molecules. These molecules can be stable or reactive intermediates. To detect these complexes spectroscopically, low temperatures are required. The molecules are embedded in an unreactive environment such as noble gas atoms which form a solid phase at temperatures near absolute zero. This technique is called matrix isolation. In many cases stable precursors are first diluted in the gas phase with a noble gas (argon, neon, nitrogen) and deposited on a cold window and then reactive intermediates can be generated by photochemical means upon irradiation with UV or visible light. These intermediates, as well as other embedded molecules, such as solvent molecules, cannot react or form complexes because of the rigidity of the matrix.

The experiments must be performed under a high vacuum to prevent contaminates from unwanted gases freezing to the cold window. Because of the broad optical transparency of the matrix material, the reactive intermediates can be detected by infrared or UV/VIS spectroscopy, but also EPR spectroscopy in case of high-spin systems.

By warming up the matrix below the boiling point of the noble gas (“annealing”), the matrix loses rigidity and reactions or the formation of aggregates are possible.

The EPR spectra can be recorded and simulated by Quantum chemical simulations. Simulations are performed to determine the parameters of the EPR spectrum and thus, to derive the properties of the observed reactive intermediate.