The phoionionization of Methyl Isocyanide, Propynal, and 2-Aminoacetonitrile molecules

Methyl isocyanide, propynal, and 2-Aminoacetonitrile are compounds of astrochemical and astrobiological interest. These molecules are the paradigm example for photochemistry which proceeds from a metastable triplet state after the latter was populated by a very rapid non radiative energy transfer from the initially populated singlet state.

Recently we have measured the threshold photoelectron and photoion spectra of these molecules as function of photon energy with high resolution, using synchrotron radiation from the DESIRS beamline of the Synchrotron Soleil. The adiabatic ionization energy has been measured using a tunable source of VUV synchrotron radiation coupled with a photoelectron photoion coincidence (PEPICO) spectrometer.

For fully understanding this ionization dynamics, one requires the characterization of the electronic ground and excited states of the neutral molecules and also of their cationic species (monomer and fragments). The assignment and the interpretation of these data require high level ab initio computations. The ionization and the appearance energies of molecules and their fragments we'll be done using explicitly correlated coupled cluster calculations taking into account the zero-point vibrational energy, core-valence and scalar relativistic effects. To further interpret the observed vibronic structure, harmonic and anharmonic frequencies we will identify the ground state of this cations.

During your visit, we propose to finalize the data treatment of the measurement issued from the above mentioned experiments, and to perform the theoretical calculations on the Methyl isocyanide, Propynal, and 2-Aminoacetonitrile neutral and ionic molecules. The goal will be to

- Assign the character of the relaxed ionic states as well as its orbital configuration.
- Estimate the adiabatic fragmentation thresholds and identify the observed fragments
- Propose the mechanisms for the unimolecular decomposition decays of these ions

At the end, we should be able to publish these results within the current year.