SEMINAIRE ISMO

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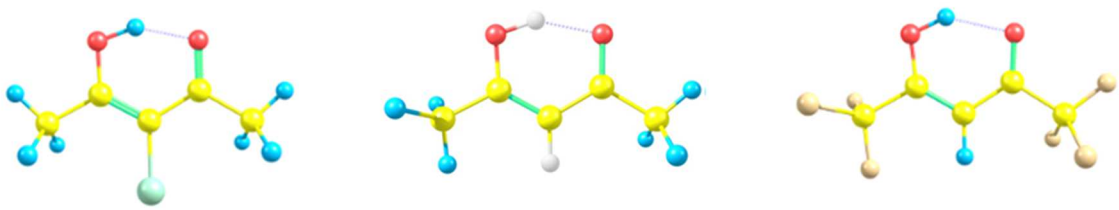
Dynamics and photodynamics of acetylacetone analogs in cryogenic matrices

Intramolecular hydrogen transfer and photo-isomerization are two of the main physico-chemical processes that often define the behavior of molecules of biological interest. In the present work we choose the β-dicarbonil family of molecules as a model system (Figure) to study the link between isotopic and electronic structure with these two processes, using vibrational and electronic spectroscopy in Neon, Nitrogen and *para*-Hydrogen matrices.

Acetylacetone: the simplest member of the β-diketone family was previously studied by our group. We will present the extension of this research which includes different analogs of acetylacetone where either the isotopic composition or the electronic structure changes. In the first case double deuterated acetylacetone was used to determine the role of the hydrogen atom from the hydroxy group in the isomer production after UV excitation. A big influence of tunnel effect in the final isomer composition of the system was found. Isomer interconversion after IR laser excitation on the first OD stretching harmonic is also discussed.

In the second part, we focus our attention in the study of structural but not electronic analogs of the original molecule, e.g.: hexafluoroacetylacetone and 3-chloro-acetylacetone. In these systems, different kinds of isomers was stabilized after electronic excitation compared to acetylacetone. In addition, the case of 2 Chloro-malonaldehyde from the smaller β-dialdehyde family will be discussed. Matrix effects, possible tunneling splitting and bandwidth-Hydrogen bond strength correlation will be also presented. Experimental results are supported with quantum chemical calculations.



β-diketone molecules: 3-Chloroacetylacetone; acetylacetone D2; Hexafluoroacetylacetone

Mardi 6 septembre 2016 à 11h

Bât. 210 – Amphi 1 (2ème étage)

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