

SEMINAIRE SPAM / LFP



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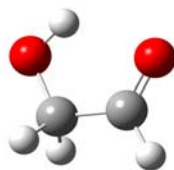
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**Le jeudi 21 janvier 2010 à 11h30
Bâtiment 522 - Salle 138**

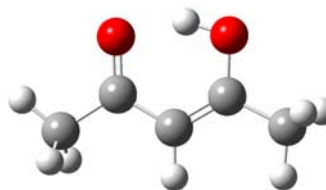
« Structure and UV isomerization of molecules with internal hydrogen bonds isolated in parahydrogen »

Molecules with internal hydrogen bond are attracting scientific attention from the beginning of the 20th century. Despite numerous theoretical and experimental studies, a number of structure and dynamic aspects, even for the smallest molecules such as Glycolaldehyde (GA) or Acetylaceton (AcAc), remains under question.

Infrared spectroscopy combined with matrix isolation technique provides a powerful tool to study various properties of molecular systems. Solid molecular hydrogen crystals with all molecules in the $J=0$ rotational state (parahydrogen, p H_2) is recently widely recognized as a very attractive media for the matrix isolation experiments. Hydrogen molecule in the $J=0$ state has anti-parallel nuclear spins resulting in absence of dipole quadruple or higher moments. Very weak interaction and "softness" of molecular hydrogen crystal results in a very small perturbation on the molecules isolated in such environment.



Glycolaldehyde



Acetylaceton

Our studies of infrared spectra of GA and AcAc isolated in p H_2 show similar patterns as those isolated in other matrices. Spectral bands are sharper in p H_2 than in other matrices. Very important feature of p H_2 is that no notable matrix split was observed. This facilitates more accurate assignment of the spectral bands which is important for the studies of conformational diversity, isomerization processes and possible hydrogen bond complexes. Experiments with added water allow us to observe and assign spectral bands of water-Ga complex. UV irradiation results in isomerization and fragmentation of GA isolated in p H_2 .

Infrared studies of AcAc revealed that the most stable structure in matrices is enol with C_s symmetry contrary to C_{2v} recently proposed in the gas phase. About 7 % of keto tautomer of AcAc was observed in the p H_2 matrices. Photoisomerization experiments using quadruple YAG radiation revealed five additional stable enolic forms of AcAc. No fragmentation was observed in the pure p H_2 matrices.

Formalités d'entrée :

Visiteur U.E. : Se faire connaître au moins 48 heures à l'avance pour l'établissement de votre autorisation d'entrée sur le Centre de Saclay.

Visiteur hors U.E. : Se faire connaître au moins 4 jours à l'avance pour les formalités d'entrée et se faire accompagner par un agent CEA.

Sans autorisation, vous ne pourrez entrer sur le Centre de Saclay. Tél. : 33.1.69.08.30.95 - Fax : 33. 1.69.08.76.39 - email : caroline.lebe@cea.fr ou veronique.gereczy@cea.fr

Dans TOUS LES CAS, se munir d'une pièce d'identité (passeport et carte d'identité - pas de permis de conduire)