

SEMINAIRE ISMO

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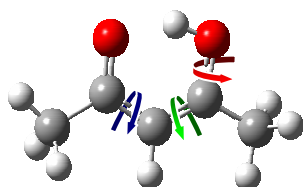
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Structure and Photodynamics of Acetylacetone Isolated In Para-Hydrogen

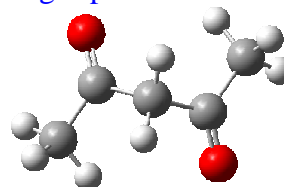
In this work we present the IR spectroscopy and UV irradiation study of Acetylacetone in solid para-hydrogen (pH₂).

Acetylacetone (AA) exists as a mixture of two tautomers: enol and keto. The enol tautomer is the most stable form in gas phase. It is stabilized by an internal hydrogen bond and has been shown to undergo proton transfer in the gas phase^[1].

Our FTIR study of AA isolated in pH₂ and DFT calculations performed at B3LYP/6-311++G(3df,3pd) level reveals that the two tautomers are trapped in the matrix, with a enol:keto ratio 96:4. This is very close to what is observed in the gas phase^[2].



Enol



Keto

In addition the enol tautomer, may be present in the pH₂ matrix as two CH₃ forms having different CH₃ orientations. This is confirmed by calculations which show that these two CH₃ rotamers have similar energies. In a Ne matrix experiment performed using the same conditions as for pH₂ only one CH₃ rotamer is observed.

UV irradiation of AA in pH₂ at 266nm results in production of 5 additional enol isomers of higher energy. This is different to what has been found in conventional matrices where only 4 isomers have been observed. This is interesting because UV irradiation of AA in the gas phase results in fragmentation of the molecule while only isomerization of AA is observed in solid matrices.

[1] G. Alagona, C. Ghio, I. J. Quantum Chem., 108, 1840 (2008)

[2] P. Y. And Spyridis G. T. , J. Am. Chem. Soc., 124, 10373 (2002)

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