



SEMINAIRE ISMO

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Elucidating bio-structures: MW spectroscopy and UV ultrafast laser vaporization

Microwave spectroscopy was originally developed as a structural technique for small molecules. However, modern rotational techniques has expanded the scope of this spectroscopy to larger biomolecular building blocks, providing accurate chemical insight on conformation, structure and molecular properties, together with benchmarking standards for theoretical calculations *in vacuo*.

In order to illustrate the possibilities of MW techniques I will present results on the conformational landscape and structural properties of several biomolecules including alkaloids, drugs and sugars. The microwave studies used a new supersonic-jet FT-MW spectrometer built at the UPV-EHU. In all cases we studied the potential energy surfaces (PES), identifying the lowest-energy conformations. Conformational energies were derived from relative intensity measurements. Finally, the effective and substitution structures were determined from the detection of multiple monosubstituted isotopologues in natural abundance (i.e., ^{13}C , ^{15}N , or ^{18}O , ranging from 0.2-1%). DFT and *ab initio* calculations were performed in all cases, evaluating the predictive performance of the MP2, B3LYP, and M06-2X methods.

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Mardi 16 octobre 2012 à 11h
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