

# High resolution mm-wave absorption spectroscopy of flexible COMs

Laboratory spectrum of 1,2-butanediol

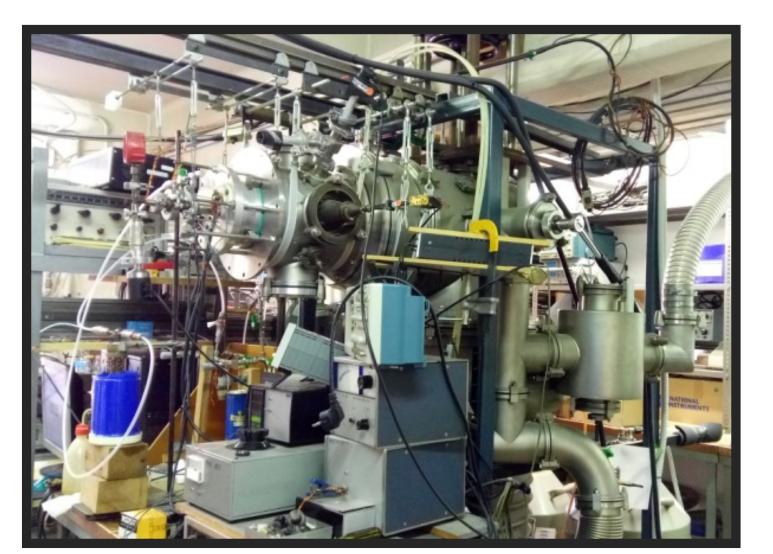
<u>Assimo Maris</u>, Sonia Melandri, Camilla Calabrese - Dipartimento di Chimica G. Ciamician - UNIBO

# WE CAN...

## **Spectrometers**

Development and Testing of New Instrumentation

... Chirped Pulsed FTMW under construction

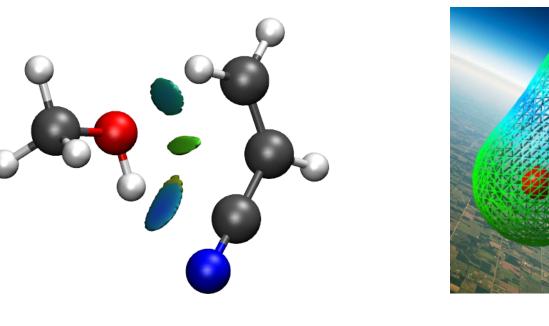


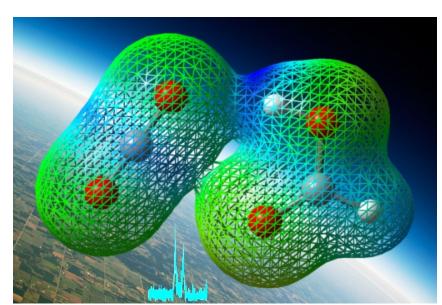
Free-Jet Absorption Millimetre Wave 50-110 GHz

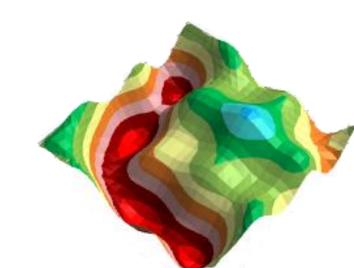
Pulsed-Jet Fourier Transform MicroWave with and without Laser Ablation, 6-18 GHz

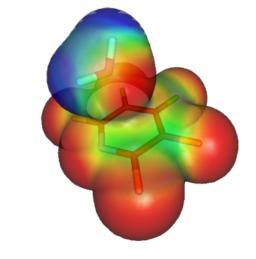
### **Quantum-mechanical simulations** for the Characterization of the Molecular and

Spectroscopic Properties: Geometry Optimizations, Potential Energy Surfaces, NBO and AIM Analysis, Anharmonic Vibrational Frequency Calculations...



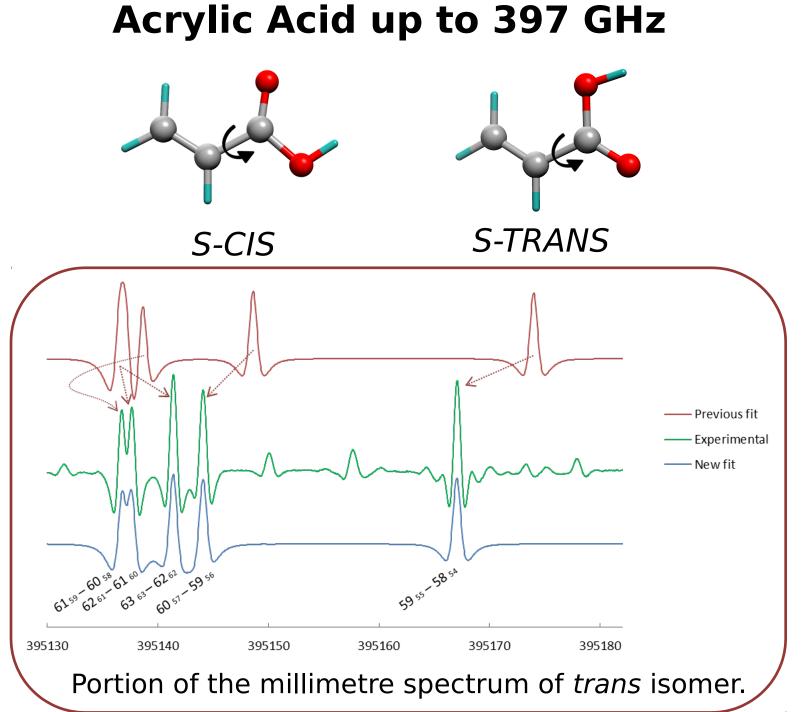




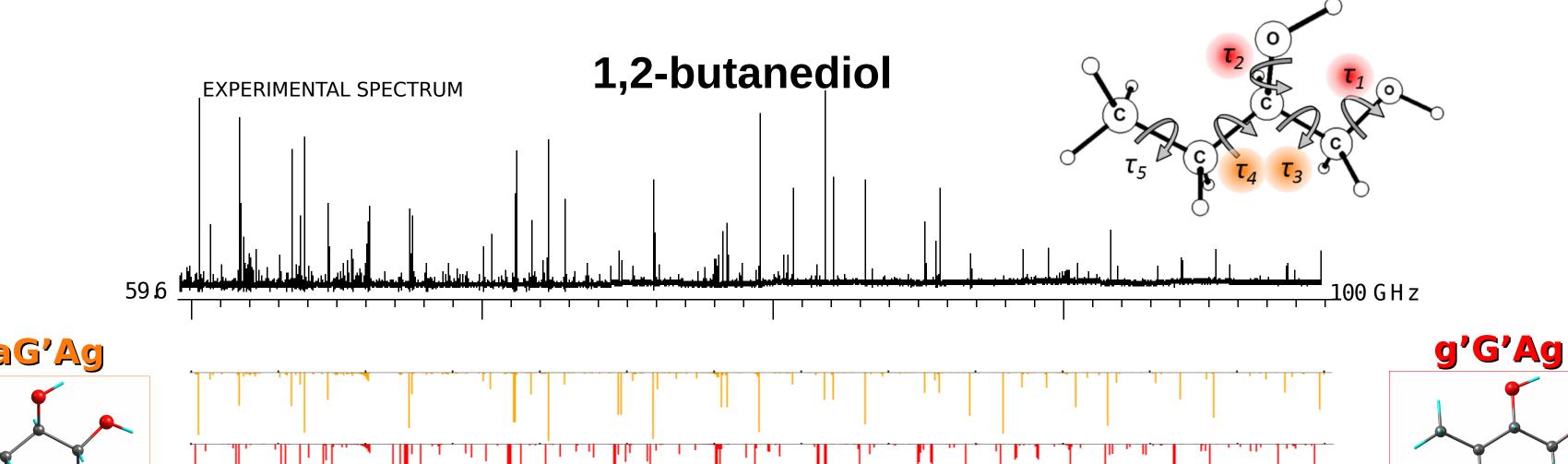


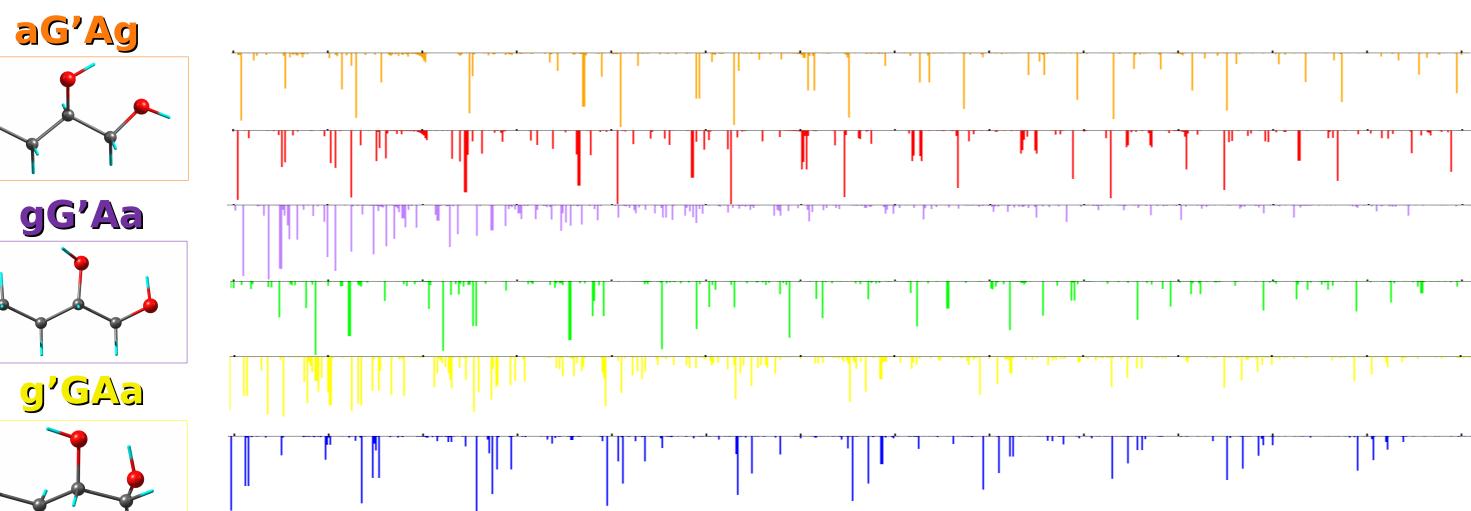
# **WE DO...**

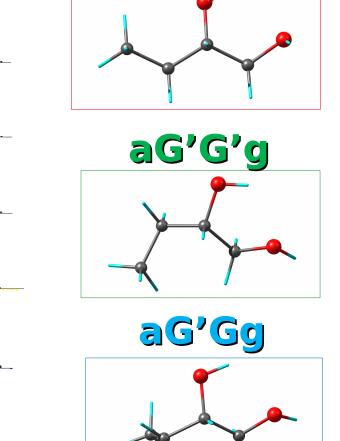
Recording and Analysis of Spectra of complex organic molecules, biomolecules, prebiotics precursors and weakly bound molecular complexes in the gas phase

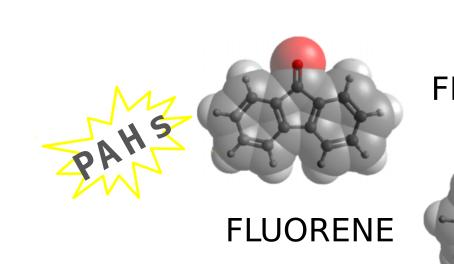


Calabrese et al. Mol. Phys., 113 (2015) 2290

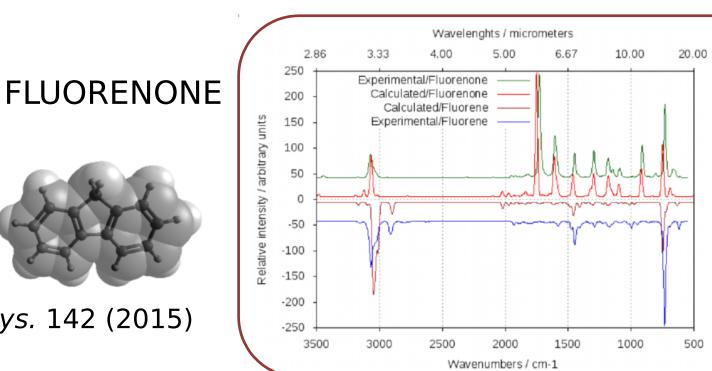




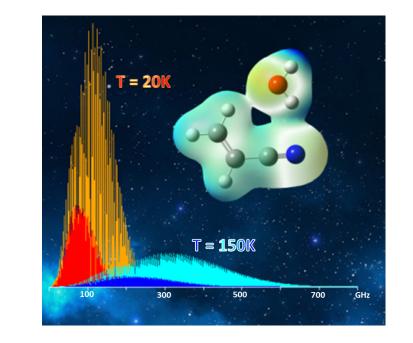


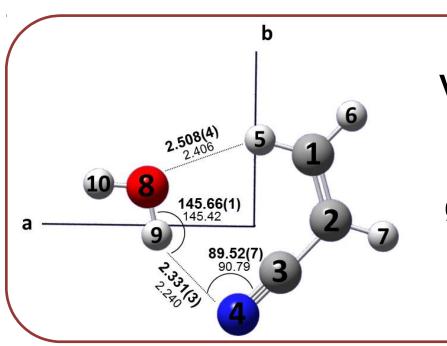


Maris et al. J. Chem. Phys. 142 (2015)



Fluorenone and Fluorene comparison between experimental and simulated mid-IR gas phase spectra (B3LYP/cc-pVTZ)





Vinyl Cyanide-Water complex  $r_{\rm e}$  and  $r_{\rm o}$  (in bold) geometries, principal inertial axes and numbering of atoms

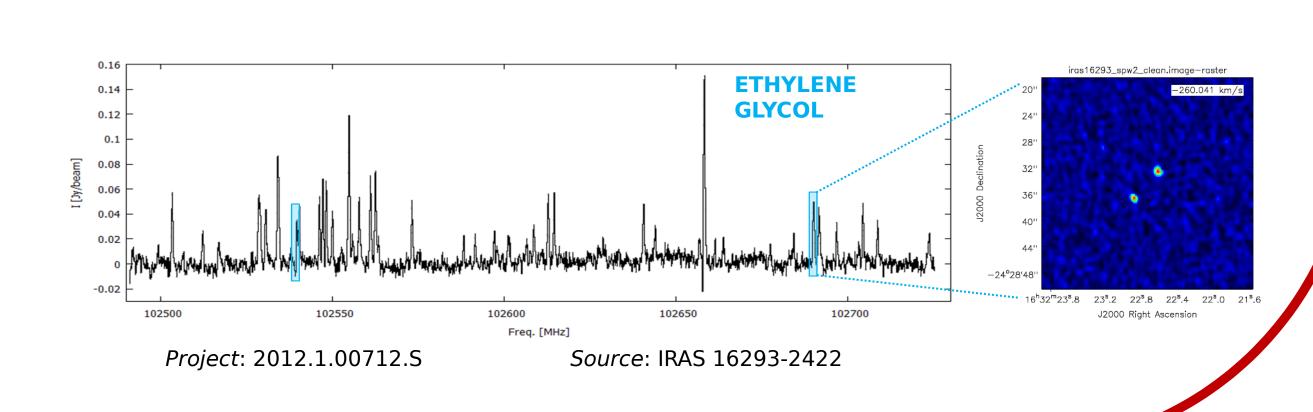
Calabrese et al. J. Phys. Chem. A, 119 (2015) 11674-11682

**Analysis of Surveys and ALMA Data** Reduction and Analysis for the recognition of molecular species in the interstellar medium









- Perform new experiments in order to extend the accurate laboratory dataset
- Exploit the advent of new telescopes able to acquire a large amount of data with increasing sensitivity and resolution
- Pursue a strong interplay between scientific communities fielding our spectroscopist skills with the astrochemical fellowship in order to deepen the understanding of the astrophysical processes which regulate the evolution of the interstellar medium

SINCE THE HIGH COMPLEXITY OF THIS FIELD WE BELIEVE THAT COLLABORATION IS THE WAY TO REACH THE GOAL

