CFEL SCIENCE

SEMINAR

13th July 2017 - 10:00

Building 99, Seminar Room I+II (EG)

Marie-Aline Martin-Drumel

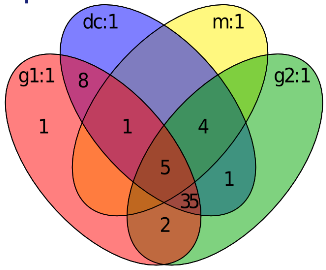
Institut des Sciences Moléculaires d’Orsay, Université Paris-Saclay, France

Characterization of new species by spectral taxonomy

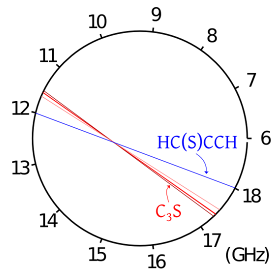
Recently it has been shown that using two stages of ion mobility it is possible to measure isomerizations - structural changes in isolated molecules. Moreover, it is Because of its structural specificity, rotational spectroscopy has great potential as an analytical tool for characterizing the chemical composition of complex gas mixtures, such as those produced by discharge in a mixture of stable precursors. However, disentangling the individual molecular constituents of a rotational spectrum, especially if many of the lines are entirely new or unknown, remains challenging and often implies theoretical calculations on species thought to be present. This search procedure is intrinsically highly biased by the initial assumption on the species present in the mixture and thus other species, potentially abundant but whose existence would not have been predicted, can remain undetected.

We are developing an empirical procedure, spectral taxonomy, to characterize and assign the transitions of the different components of a mixture without any a priori knowledge on their atomic composition or structure. The procedure requires the acquisition of the rotational spectrum of a rich mixture in a wide spectral region (for instance using chirped-pulse techniques) revealing the transitions of the polar species present without any bias. These lines are subsequently categorized based on their relative intensities under series of assays: removal of a precursor, application of an external a magnetic field, eventually removal of the excitation source (discharge, laser, thermal heating etc.), eventually followed by double resonance tests to link all transitions sharing energy levels.

Initially developed in the microwave spectral region, where the approach combines the complementary strengths of two techniques, broadband chirped-pulse Fourier-transform microwave spectroscopy and narrowband cavity Fourier-transform microwave spectroscopy, the technique allowed to detect new vibrational satellites of previously known transient species [C2S, C3S, c-C3H2, AlS,...] as well as several entirely new compounds [HC(S)CCH, HC(O)C4H, CH3SNO, GeCn,...]. The method is currently implemented in the millimeter and submillimeter regions where it matches perfectly the actual interstellar observations, for instance by the ALMA telescope.



Example of Categorization of 57 transitions observed on the CP spectrum of a mixture of C_2H_2 and CS_2. Dependences: C_2H_2 (g1), CS_2 (g2), discharge (dc), magnet (m)



DR matches in the [dc:1,m:0,g1:1,g2:1] category (discharge lines, non-magnetic, depend on both gases) that allowed detection of HC(S)CCH

References

[1] K. N. Crabtree, M.-A. Martin-Drumel, G. G. Brown, S. A. Gaster, T. M. Hall, M. C. McCarthy, J. chem. Phys. 144, 124201 (2016)

Host: Melanie Schnell - CFEL Molecular Physics seminar