ANALYSIS OF THE ROTATIONAL SPECTRUM OF LARGE DIFLUOROMETHANE CLUSTERS

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In the last few years the development of chirp pulsed Fourier transform microwave (CP-FTMW) spectrometers has enables the studies of relatively large rotors and observations of molecular clusters that were difficult to detect previously. In this work we present the study of large oligomers of difluoromethane ($(CH_2F_2)_n$, with n from 5 to 7) for which experimental measurements were obtained during a collaboration between different research groups (especially at the University of Virginia – USA[c] and Universidad del País Vasco – Spain[d]). State-of-the-art quantum chemical calculations and structural results for the molecular species will be presented. The challenging decomposition of the spectrum into the individual rotational spectra for each species presented in the jet expansion will be carried out. In particular the approach using AUTOFIT algorithm[e] running on Amazon Web Service (AWS) and High Performance Computing (HPC) systems and its modified version for large molecular system will be presented.

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[c] Broadband Fourier transform rotational spectroscopy for structure determination: The water heptamer. C. Perez et al. Chem. Phys. Lett. 571 (2013) 1-15.

[d] Structural Studies of Nicotinoids: Cotinine versus Nicotine. I. Uriarte et al. Chem. Eur. J. 23 (2017) 7238 -7244.

[e] AUTOFIT, an automated fitting tool for broadband rotational spectra, and applications to 1-hexanal. N.A. Seifert et al. J. Mol. Spectrosc. 312 (2015) 13-21.