Contribution ID: **55** Type: **Poster**

Theoretical infrared Spectrum of the Ethanol Hexamer

Experimental infrared spectrum of a sample is used to characterize different compounds that are present in the sample. Two different compounds will always have different infrared spectra. For a compound with several isomers, the experimental spectrum will be a combination of the spectra of different possible isomers. It is not possible to determine these possible isomers experimentally. Using computational chemistry, one can locate these isomers and compute their theoretical infrared spectra. Combining the theoretical and the experimental spectra, one can then be able to identify different isomers that can contribute to the experimental sample. In this work, we applied this procedure to determine the structures of the ethanol hexamer that could contribute to the population of the cluster. We started by sampling different isomers which have been optimized at the APFD/6-31++G(d,p) level of theory. 139 different isomers have been located [1]. From the 139 APFD optimized isomers, we selected 98 for further optimization at the MP2/aug-cc-pVDZ level of theory for the accuracy of the results. Frequencies calculation for all the isomers is performed at the MP2/aug-cc-pVDZ level of theory. For one isomer, about 70 hours have been used on an Intel® Xeon® 24 cores, 2.6 GHz and 128 GB memory at CHPC to compute the frequencies and their intensities. The computed frequencies, as well as their intensities, are used to produce the theoretical spectra of the isomers. Then we used the infrared spectra of these possible isomers weighted by their canonical probability to produce a unique theoretic infrared spectrum of the ethanol hexamer using Voigt profiles [2]. The computed theoretical spectrum is in qualitative agreement with the experimental spectrum of the ethanol hexamer [3].

Supported Student

Primary author: MALLOUM, Alhadji (University of the Free State)

Co-authors: Prof. FIFEN, Jean Jules (The University of Ngaoundere); CONRADIE, Jeanet (University of the Free State)

Presenter: MALLOUM, Alhadji (University of the Free State)

Session Classification: SIG Poster

Track Classification: SIG Seminar: Chemistry, Material Science and Health Science