Chiral Molecular Interactions: Jet-Cooled Rotational Spectroscopy and Quantum Chemistry Calculations

Yunjie Xu

Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada, T6G 2G2

Abstract: Our research program is dedicated to exploring mechanisms of chirality recognition, transfer, and amplification at the molecular level. To investigate chirality recognition and transfer, we apply jet-cooled rotational spectroscopy alongside quantum chemistry calculations to examine rotational spectra of selected chiral molecules, as well as their hydrates and aggregates, recorded in a supersonic jet expansion.

In this presentation, we will first explore how stepwise solvation, i.e., adding one water molecule at a time, influences the conformational landscape of an example chiral alcohol.[1] We aim to highlight the connection between the low-temperature, gas-phase investigations of small hydrated chiral molecular clusters and the solvation effects in a bulk environment.[2] Next, we will demonstrate chirality-controlled structural properties and tunneling dynamics in a prototype chiral molecular pair.[3] Additionally, we will address the potential practical application of using rotational spectra of such chiral molecular contact pairs to determine enantiomeric excess of a chiral sample.

Generally, the high resolution and high sensitivity of the cavity-based and chirped-pulse Fourier transform rotational spectroscopic techniques offer conformer specific information on chiral molecular systems, as well as detailed evidence of large amplitude motions. Such specific experimental data, rarely obtainable by other spectroscopic techniques, provide deeper insights into the mechanisms of the chiral events.

References:

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