

Physical Chemistry Seminar

Tuesday,
October 13, 2015

11:00 am

Room 1315
Chemistry Building

Spectral Signatures of Chirality, Chirality Recognition, and Chirality Transfer



Professor Yunjie Xu
*Department of Chemistry
University of Alberta, Canada*

Host: Etienne Garand

Chirality, or “handedness”, represents an intrinsic property of life. Our research focuses on applying and developing new spectroscopic tools to determine chirality and to establish chirality recognition models at the molecular level. In this presentation, I will first speak about high resolution spectroscopic studies of chirality recognition in several hydrogen-bonded clusters containing small transient chiral fluoroalcohols using both the cavity-based and chirped-pulse Fourier transform microwave techniques. Second, chiroptical spectroscopy, such as vibrational circular dichroism (VCD), can provide not only rich structural information of chiral molecules in solution, but also important insights into how they interact with each other and with solvent molecules. Our VCD results on transition metal complexes and amine borane complexes in solution highlight the unique VCD sensitivity to solvent effects and hydrogen-bonding interactions. I will focus on water molecules which are closest to a chiral molecule in aqueous solution and our proposed “clusters-in-a-liquid” approach for simulating chiroptical spectra in water. The link between VCD spectral signatures of small hydration clusters and those obtained in aqueous solution will be discussed.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students can meet with the speaker at 1:00 pm in Room 8305F