CHIRALITY RECOGNITION/TRANSFER/AMPLIFICATION: ROTATIONAL SPECTROSCOPIC AND CHIROPTICAL SPECTROSCOPIC STUDIES

YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*.

A molecule is chiral if its mirror image cannot be superimposed onto itself. Chirality serves an essential function in life. Our research program centres on understanding mechanisms of chirality recognition/transfer/amplification at the molecular level. To achieve this goal, we apply and develop new spectroscopic tools to characterize structural and dynamical properties of chiral molecules and non-covalent interactions among them in the gas phase, solution, cold rare gas matrices and at liquid-liquid interfaces. In particular, we emphasize the connection between the gas phase results obtained by using high resolution spectroscopy with those obtained in the condense phases. In the first example, we investigate tetrahydro-2-furoic acid, a chiral carboxylic acid, using broadband chirped pulse-Fourier transform microwave spectroscopy. Aided by a semiempirical quantum chemistry code for conformational search and DFT calculations, we examine its conformational landscape and chirality recognition in its binary adducts. The unusual conformational distributions and chirality controlled conformational preferences will be discussed. We further investigate the acid in cold rare gas matrices and as a liquid using vibrational circular dichroism to extract dominant species under these conditions. In the second example, I will discuss extremely strong chirality transfer from a chiral nickel complex to solvent molecules detected as Raman optical activity. We propose a chirality transfer/amplification mechanism based on quantum plasmons, i.e. plasmons in the few-atom limit. The interplay between experiment and theory is essential for all the work described.