USING COMPUTATIONAL TOOLS TO ENHANCE LEARNING IN AN UNDERGRADUATE MOLECULAR SPECTROSCOPY COURSE

M. REZA POOPARI, SHYAM PARSHOTAM, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*.

In molecular spectroscopy, our models of the molecular world are built on rigorous spectroscopic experimentation and rich interplay between theory and experiment. To instill such appreciation to undergraduate students, who have little experience in either spectroscopic experiments and theory, is challenging. We have developed a new computational laboratory component to complement the material covered in a senior undergraduate course on molecular spectroscopy. Specifically, we focus on illustrating molecular spectroscopic concepts (some of which can be quite abstract and complicated) taught in class with electronic structure calculations. This talk will describe our implementation and the learning outcome. Two particular examples will be discussed. One is related to the misconception that electron density is the main factor responsible for NMR chemical shifts and how we utilize both experimental data and calculations to help students overcome this common misconception. The other deals with differences in geometries, for example, those obtained using rotational constants directly, isotopic substitution procedures, and electronic structure calculations. This talk will also discuss how the above activities worked in practice and the improvements we plan to implement next time.