Applications of Vibrational Spectroscopy to Current Problems in Molecular Structure

Vibrational spectroscopy is a branch of molecular spectroscopy used to probe and, ultimately, understand the structure of molecules. When using this technique, especially when it is combined with quantum mechanical calculations, we can gain a better insight into how the structure of a molecule affects what is seen in vibrational (infrared and Raman) spectra; or, conversely, we can use a molecule’s unique vibrational spectrum to determine its structure. Understanding the geometry and lowest energy, i.e. most stable, structure of a molecule is particularly important when investigating the structural preference(s) of a substance which may have several possible conformational isomers. First, I will discuss how the combination of molecular spectroscopy and quantum mechanical calculations were used in our structural and conformational study of fluoroacetyl chloride. Additionally, a brief discussion will be given on one of our current projects, which involves applying infrared spectroscopy and quantum mechanical calculations to determine structural changes in phosphoenolpyruvate when it binds to the enzyme, human liver pyruvate kinase.