FINGERPRINTS OF INTRAMOLECULAR HYDROGEN BONDS: SYNCHROTRON-BASED FAR IR STUDY OF THE CIS AND TRANS CONFORMERS OF 2-FLUOROPHENOL

AIMEE BELL, JAMES SINGER, JENNIFER VAN WIJNGAARDEN, Department of Chemistry, University of Manitoba, Winnipeg, MB, Canada.

Rotationally-resolved vibrational spectra of two planar conformers of 2-fluorophenol have been collected from 100-1000 cm\(^{-1}\) using the Bruker IFS125HR FTIR spectrometer at the Canadian Light Source with a resolution of 0.000959 cm\(^{-1}\). The cis conformer is lower in energy by 2.9 kcal/mol (MP2/aug-cc-pvDZ) and is thought to be stabilized by an intramolecular hydrogen bond between the hydroxyl group and neighbouring fluorine atom on the ring. The OH out-of-plane torsion bands below 400 cm\(^{-1}\) provide the best fingerprint to distinguish between the two conformers in the gas phase spectrum as the \(c\)-type band origin of the cis conformer is blue-shifted by 36 cm\(^{-1}\) from that of the trans conformer as result of the intramolecular interaction. In this talk, we will discuss the progress of the analysis of this complex far infrared spectrum of 2-fluorophenol.