

Computational and Spectroscopic Studies of SO₂-Formic Acid Complexes

Bronwyn Harrod and John W. Keller

Department of Chemistry and Biochemistry, University of Alaska Fairbanks

Fairbanks, AK, 99775-6160

SO₂ and formic acid occur in interstellar and planetary environments. The purpose of this study was to computationally predict the existence of one or more complexes between these two molecules, and then attempt to experimentally identify them using infrared spectroscopy. For the computational aspects of the study, *HyperChem* and *Gaussian 03* were utilized. Calculations were carried out using semiempirical, HF, and DFT B3LYP methods, with basis sets ranging from 6-31G(d,p) to cc-pVDZ. Two weakly-bound but stable complexes were identified. The form with the O-H---O hydrogen bond was calculated to be more stable than the C-H---O bonded complex. Gas phase infrared spectroscopy was used to analyze SO₂ and formic acid vapor separately, then a spectrum of the mixture was obtained. Numerical analysis of spectra attained under low pressure conditions has not yet revealed any unique complex vibrations. Further experiments using higher gas pressures and a short pathlength cell are underway.