DETERMINATION OF THE RATE OF TRANSFORMATION OF FORMAMIDE DIMERS AND RESOLVED SPECTRA OF FORMAMIDE DIMERS

Mike Cato, Devashis Majumdar and Jerzy Leszczynski

Jackson State University, Interdisciplinary Center for Nanotoxicity, Jackson, MS 39217, USA

Abstract: Four singly and doubly hydrogen bonded formamide dimers, six trans-trans and five trans-cis formic acid dimers are investigated at the correlated level of quantum chemistry theory using coupled cluster with singles and doubles with a 6-31G++(d,p) split valence basis set. Harmonic vibrational frequencies and IR intensities of the intermolecular modes in the four possible formamide dimer systems and the formamide molecule itself were determined. The Amide I vibrational mode and Amide II vibrational mode were examined for all structures. Anharmonic vibrational modes were determined for all structures, the rate of transformation of various formamide dimers was determined and the vibrationally resolved spectra for the formamide structures were calculated.