Structure And Vibrational Analysis Of Ethyl 3-Amino-2-Butenoate

A. R. Berenji, S. F. Tayyari, M. Vakili, M. Jamialahmadi
Department of Chemistry, Ferdowsi University of Mashhad, Mashhad 91779, Iran
Presenting author: berenji@staff.um.ac.ir, aberenji@gmail.com

Molecular structure and vibrational spectra of ethyl 3-amino-2-butenoate (EAB) were investigated using density functional theoretical (DFT) calculations. The geometrical parameters and vibrational wavenumbers were obtained at the B3LYP/6-311++G(d,p) level. The results were compared with the corresponding experimental infrared (IR) and Raman spectra. Fourier Transform IR and Raman spectra of EAB were clearly assigned. The spectra were also compared with two similar molecules, namely methyl 3-amino-2-butenoate (MAB) [1] and 4-amino-3-penten-2-one (APO) [2]. The theoretical calculations show that the intramolecular hydrogen bond strength of EAB is the same as that of MAB and weaker than that of APO, which is in agreement with the spectroscopic results. Furthermore, the IR spectra of EAB (as neat and in CCl_4 solutions) indicate that EAB (the same as MAB) is engaged in an intermolecular hydrogen bond.

References

1. A. R. Berenji, S. F. Tayyari, M. Rahimizadeh, H. Eshghi, M. Vakili, and A. Shiri, Spectrochim. Acta A **102**, 350 (2013).
2. S. F. Tayyari, H. Raissi, and F. Tayyari, Spectrochim. Acta A **58**, 1681 (2002).

Keywords: β-Enaminones, Ethyl 3-aminocrotonate, Vibrational spectra, Intramolecular hydrogen bond, DFT