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Experimental and DFT dimer modeling studies of the H-bond induced-vibration modes of L-β-Homoserine

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Abstract

The vibrational spectra for L-β-Homoserine have been measured (IR absorption: 4000 – 400 cm^{-1}/Raman spectra: 4000 – 200 cm^{-1}). Characteristic vibrational modes of ammonium ($-NH_3^+$), carboxylate ($-CO_2^-$) and hydroxyl (−OH) groups across the 3700 – 1400 cm^{-1} are all identified to have originated in *inter*-molecular hydrogen bonding involving these functional groups. DFT calculations at B3LYP/6-311++G(d, p) level have yielded a single neutral monomer in the gas phase. Since as a member of the amino acids which are known to possess zwitterionic structure in condensed phase, the neutral monomer of L-β-Homoserine is optimized to a zwitterionic structure in a water medium. Consideration of two dimer structures, one dimer with –N–H···O bond and another –O–H···O bond, has given rise to vibrational modes that satisfactorily fit to all the observed absorption and Raman bands. It is found that the dimer with –O–H···O bond (binding energy, 8.896 kcal/mol) is more tightly bound than the dimer with –N–H···O bond (8.363 kcal/mol).

Keywords : L-β-Homoserine, IR, Raman, DFT, Zwitterion, N−H···O and O−H···O *inter*-molecular hydrogen bonding