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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 ($-\text{NH}_3^+$), carboxylate ($-\text{CO}_2^-$) and hydroxyl ($-\text{OH}$) 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 $-\text{N}-\text{H}\cdots\text{O}$ bond and another $-\text{O}-\text{H}\cdots\text{O}$ 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 $-\text{O}-\text{H}\cdots\text{O}$ bond (binding energy, 8.896 kcal/mol) is more tightly bound than the dimer with $-\text{N}-\text{H}\cdots\text{O}$ bond (8.363 kcal/mol).

Keywords : L- β -Homoserine, IR, Raman, DFT, Zwitterion, $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ *inter*-molecular hydrogen bonding

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