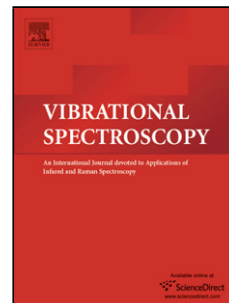


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Surface enhanced Raman scattering of neutral and zwitterionic α - and β -Proline monomers adsorbed on Au_3 cluster: A DFT study

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Abstract

Density functional theory (DFT) based energetics and surface enhanced Raman spectra of Au_3 tagged neutral and zwitterionic states of both α and β -Proline monomers are investigated to gain molecular level understanding in detection of the amino acids. Raman enhancement of vibrational modes is significant when the cluster interacts with the Proline systems through energetically less preferential orientation of the monomers. While methylene stretching, N-H rocking and stretching modes of C=O and O-H bonds are important for recognition of the neutral systems, methylene stretching, the asymmetric stretching, wagging and scissoring modes of vibrations of NH_2^+ and asymmetric stretching of $\text{O}=\text{C}=\text{O}^-$ play prominent role in detection of zwitterionic systems. Justification for observed trends comes from the molecular polarizability, depolarization ratio of the vibrational modes, enhancement factors of the modes calculated based on the static Raman intensities and NBO analysis of stabilizing interactions.

Keywords: α -, β -Proline, Au_3 cluster, Raman Scattering, Depolarization ratio, Enhancement Factor, NBO

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