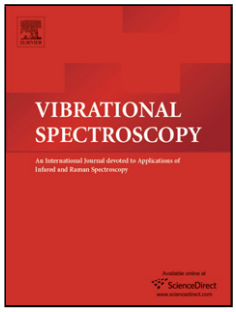

Title: Surface enhanced Raman scattering of neutral and zwitterionic α- and β-Proline monomers adsorbed on Au_3 cluster: A DFT study

Author: N V Suresh Kumar

PII: S0924-2031(18)30082-1
DOI: https://doi.org/doi:10.1016/j.vibspec.2018.06.008
Reference: VIBSPE 2810

To appear in: *VIBSPE*

Received date: 3-3-2018
Revised date: 23-5-2018
Accepted date: 14-6-2018

Please cite this article as: N V Suresh Kumar, Surface enhanced Raman scattering of neutral and zwitterionic *rmalpha-* and *rmbeta*-Proline monomers adsorbed on Au_3 cluster: A DFT study, *<![CDATA[Vibrational Spectroscopy]]>* (2018), https://doi.org/10.1016/j.vibspec.2018.06.008

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

N V Suresh Kumar[1]

Center for Computational Natural Sciences and Bioinformatics (CCNSB), International Institute of Information Technology, Hyderabad - 500 032, India.

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 $O{=}C{=}O^-$ 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

*N V Suresh Kumar

Email address: nvs.kumar@iiit.ac.in (N V Suresh Kumar)

[1]Center for Computational Natural Sciences and Bioinformatics (CCNSB), International Institute of Information Technology, Hyderabad - 500 032, India and Department of Physics, Koneru Lakshmaiah Education Foundation, Green fields, Vaddeswaram, Guntur - 522 502, India, Tel.: +91 9848985146