

Paper Title :- Vibrational spectra of distorted structure Macro & Nano molecules: An algebraic approach

Name of the Journal: - Biophysical Chemistry

Author's:- Srinivasa Rao Karumuri, Jalaparthy Vijayshekar, Velagapudi Uma Maheswara Rao, Gan-ganagunta Srinivas, Aappikatla Hanumaiah

ABSTRACT

Using the Lie algebraic method the vibrational frequencies of 97 resonances Raman lines ($A_{1g} + B_{1g} + A_{2g} + B_{2g}$) and 38 infrared bands (E_u) of octaethylporphyrinato-Ni (II) and its mesodeuterated and ^{15}N -substituted derivatives and Fullerenes C_{60} and C_{70} of 7 vibrational bands are calculated using $U(2)$ algebraic Hamiltonian with four fitting algebraic parameters. The results obtained by the algebraic technique have been compared with experimental data; and they show great accuracy.

Keywords: Lie Algebra; Vibrational Spectra; Ni (OEP); Ni (OEP)-d₄ & Ni (OEP)-N₄ and Fullerenes