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S. Muthu, E. Elamurugu Porchelvi

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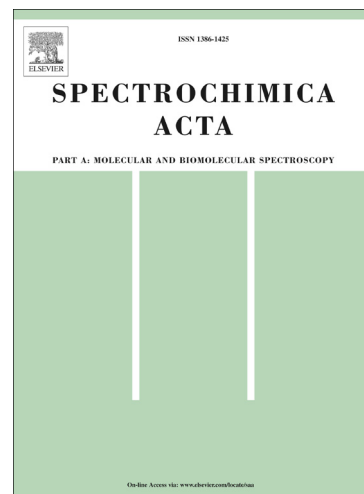
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## Experimental Spectroscopic (FTIR, FT-Raman, FT-NMR, UV-Visible) and DFT Studies of 1-ethyl-1, 4-dihydro-7-methyl-4oxo-1, 8 naphthyridine-3-carboxylic acids

S.Muthu<sup>1\*</sup>, E.Elamurugu Porchelvi<sup>2</sup>

<sup>1</sup>Department of physics, Sri Venkateswara College of Engg, Sriperumbudur-602105, Tamilnadu, India. Tamilnadu, India.

<sup>2</sup>Department of physics, Kanchi Pallavan Engineering College, Kanchipram-631502, Tamilnadu, India.

Corresponding author, Tel.: 919443690138.

Email address: [muthu@svce.ac.in](mailto:muthu@svce.ac.in) (S.Muthu)

### Abstract

The solid phase FTIR and FT-Raman spectra of 1-ethyl-1, 4-dihydro-7-methyl-4oxo-1,8 naphthyridine-3-carboxylic acid (EDMONCA) have been recorded in the regions 4000-500 and 4000-400 $\text{cm}^{-1}$  respectively. The equilibrium geometry, harmonic vibrational frequencies have been investigated by DFT/B3LYP and B3PW91 methods with 6-311G (d,p) basis set. The difference between the observed and scaled wave number values of most of the fundamentals is very small. The assignments of the vibrational spectra have been carried out with the aid of normal coordinate analysis (NCA) following the scaled quantum mechanical force field methodology (SQMFFM). Stability of the molecule arising from hyper conjugative interactions, charge delocalization has been analyzed using natural bond orbital (NBO) analysis. UV-visible spectrum of the compound was recorded and the electronic properties HOMO and LUMO energies were measured. The electric dipole moment ( $\mu_D$ ) and first hyperpolarizability ( $\beta_{tot}$ ) values of the investigated molecule were computed using ab initio quantum mechanical calculations. The calculated results also show that the EDMONCA molecule may have

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