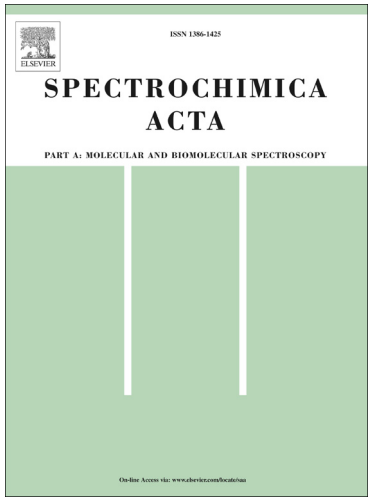
Accepted Manuscript



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

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PII: S1386-1425(13)00753-1
DOI: http://dx.doi.org/10.1016/j.saa.2013.07.016
Reference: SAA 10760

To appear in: *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*

Received Date: 4 May 2013
Revised Date: 30 June 2013
Accepted Date: 16 July 2013

Please cite this article as: S. Muthu, E. Elamurugu Porchelvi, Experimental Spectroscopic (FTIR, FT-Raman, FT-NMR, UV-Visible) and DFT Studies of 1-ethyl-1, 4-dihydro-7-methyl-4oxo-1, 8 napthyridine-3-carboxylic acids, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2013), doi: http://dx.doi.org/10.1016/j.saa.2013.07.016

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

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Abstract

The solid phase FTIR and FT-Raman spectra of 1-ethyl-1, 4-dihydro-7-methyl-4oxo-1,8 napthyridine-3-carboxylic acid (EDMONCA) have been recorded in the regions 4000-500 and 4000-400cm^{-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 different between the observed and scaled wave number values of most of the fundamental 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 LOMO energies were measured. The electric dipole moment (μ_D) and first hyperpolarizability (β_{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