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Synthesis, Structural, Spectroscopic and Nonlinear Optical Properties of New Picolinate Complex of Manganese (II) Ion

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Abstract : Novel picolinate complex of manganese(II) ion, [Mn(pic)2] [pic: picolinate or 2-pyridinecarboxylate], was prepared and fully characterized by single crystal X-ray structure determination. The manganese(II) complex was characterized by FT-IR, FT-Raman and UV–Vis spectroscopic techniques. The C=O, C=N and C=C stretching vibrations were found to be strong and simultaneously active in IR and spectra. In order to support these experimental techniques, density functional theory (DFT) calculations were performed at Gaussian 09W. Although the supramolecular interactions have some influences on the molecular geometry in solid state phase, the calculated data show that the predicted geometries can reproduce the structural parameters. The molecular modeling and calculations of IR, Raman and UV-vis spectra were performed by using DFT levels. Nonlinear optical (NLO) properties of synthesized complex were evaluated by the determining of dipole moment (μ), polarizability (α) and hyperpolarizability (β). Obtained results demonstrated that the manganese(II) complex is a good candidate for NLO material. Stability of the molecule arising from hyperconjugative interactions and charge delocalization was analyzed using natural bond orbital (NBO) analysis. The highest occupied and the lowest unoccupied molecular orbitals (HOMO and LUMO) which is also known the frontier molecular orbitals were simulated, and obtained energy gap confirmed that charge transfer occurs within manganese(II) complex. Molecular electrostatic potential (MEP) for synthesized manganese(II) complex displays the electrophilic and nucleophilic regions. From MEP, the the most negative region is located over carboxyl O atoms while positive region is located over H atoms.

Keywords : DFT, picolinate, IR, Raman, nonlinear optic
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