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Conventional and Computational Investigation of the Synthesized Organotin(IV) Complexes Derived from o-Vanillin and 3-Nitro-o-Phenylenediamine

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Abstract : Schiff base with general formula H_2L was derived from condensation of o-vanillin and 3-nitro-o-phenylenediamine. This Schiff base was used for the synthesis of organotin(IV) complexes with general formula R_2SnL [R=Phenyl or n-octyl] using equimolar quantities. Elemental analysis UV-Vis, FTIR, and multinuclear spectroscopic techniques (^1H, ^{13}C, and ^{119}Sn) NMR were carried out for the characterization of the synthesized complexes. These complexes were coloured and soluble in polar solvents. Computational studies have been performed to obtain the details of the geometry and electronic structures of ligand as well as complexes. Geometry of the ligands and complexes have been optimized at the level of Density Functional Theory with B3LYP/6-311G (d,p) and B3LYP/MPW1PW91 respectively followed by vibrational frequency analysis using Gaussian 09. Observed ^{119}Sn NMR chemical shifts of one of the synthesized complexes showed tetrahedral geometry around Tin atom which is also confirmed by DFT. HOMO-LUMO energy distribution was calculated. FTIR, ^1HNMR and $^{13}CNMR$ spectra were also obtained theoretically using DFT. Further IRC calculations were employed to determine the transition state for the reaction and to get the theoretical information about the reaction pathway. Moreover, molecular docking studies can be explored to ensure the anticancer activity of the newly synthesized organotin(IV) complexes.

Keywords : DFT, molecular docking, organotin(IV) complexes, o-vanillin, 3-nitro-o-phenylenediamine
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