DETERMINATION OF STRUCTURAL AND ELECTRONIC PARAMETERS OF ANTIMONY COMPLEX, FROM THEORETICAL CALCULATIONS

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In this study, ground states of antimony (Sb\(^{\text{V}}\)) with organic ligands complexes were studied by using density functional theory hybrid methods in order to obtain structural, electronic and vibrational spectral parameters. The mapping molecular electrostatic potential surface of the molecules computed to information about the charge density distribution of the molecules and its chemical reactivity. Frontier molecule orbital properties, HOMO and LUMO energies, global descriptors, and the total density of state diagram analysis were performed by using the time-dependent density functional theory. For the learning nonlinear optical properties, polarizability and hyperpolarizability tensors of the molecule were calculated.