P 37. THEORETICAL INVESTIGATIONS ON FIRST AND SECOND FRONTIER MOLECULAR ORBITALS AND VERTICAL TRANSITION ENERGIES OF TRIFLUOROMETHYL CONTAINING STILBENE DERIVATIVE

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ABSTRACT: The theoretical calculations on the molecular orbital structure and linear optical properties of trifluoromethyl containing stilbene derivative can provide useful information for the design of new efficient materials. The one-photon absorption (OPA) characterizations of the title molecule have been thoretically obtained by density functional theory (DFT) at B3LYP level. To understand the phenomena in the context of molecular orbital picture; on the basis of optimized geometries, the highest occupied molecular orbitals (HOMO), the lowest unoccupied molecular orbitals (LUMO) and the HOMO-LUMO band gaps for the examined compound have been evaluated by DFT.

Keywords: One-Photon Absorption, Vertical Transition Wavelength, Computational Studies, HOMO-LUMO Energies, Density Functional Theory