

**P 31. COMPUTATIONAL STUDY ON DIPOLE POLARIZABILITIES AND ONE-PHOTON ABSORPTION WAVELENGTHS OF ETHYLENIC LINKAGE WITH DONOR-ACCEPTOR SUBSTITUENTS**

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**ABSTRACT:** To understand linear optical characterization of an ethylenic linkage with donor-acceptor substituents, we have computed the one-photon absorption (OPA) wavelengths and static linear polarizability utilizing density functional theory (DFT). The OPA and dispersion-free dipole polarizability results have been found to be rather adequate for assessing connectivities between the electronegativities of donor-acceptor groups and linear optical properties. Using DFT at B3LYP level, one can obtain a reasonably accurate description of the optical spectrum and static linear polarizability of the studied structure.

*Keywords: Linear Optics, One-Photon Absorption, Static Dipole Polarizability, Ethylenic Linkage, Donor-Acceptor Substituents.*