P 33. DFT METHODOLOGIES FOR COMPUTING DIPOLE POLARIZABILITIES, FIRST AND SECOND FRONTIER MOLECULAR ORBITAL ENERGIES OF METHYL-3-(P-NITROPHENYL) CARBAZATE

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ABSTRACT: To reveal the linear optical properties of methyl-3-(p-nitrophenyl) carbazate, density functional theory (DFT) calculations have been carried out to compute the static dipole polarizability tensor components. As the static dipole polarizability values depend on the DFT functional used, we carried out the computation of dispersion-free linear polarizability at the DFT level using B3LYP method. The highest occupied molecular orbitals (HOMO), the lowest unoccupied molecular orbitals (LUMO) and the HOMO-LUMO band gaps for the title compound have been also examined by DFT/ B3LYP procedure.

Keywords: Linear Optics, Static Linear Polarizability, First Frontier Molecular Orbitals, Second Frontier Molecular Orbitals, Density Functional Theory