P 8. COMPUTATIONAL STUDIES ON ELECTRIC DIPOLE MOMENT AND QUADRATIC HYPERPOLARIZABILITY OF (5-BROMOPYRIDINE-2,3-DIYL)BIS(SALICYLIDENEAMIN)

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ABSTRACT: To investigate the linear optical and microscopic second-order nonlinear optical (NLO) behaviour of (5-bromopyridine-2,3-diyl)bis(salicylideneamin), we have computed the electric dipole moment and dispersion-free quadratic hyperpolarizability values using density functional theory (DFT). The calculated non-zero electric dipole moment value shows that the title compound might have first hyperpolarizability with non-zero value. The highest occupied molecular orbitals (HOMO), the lowest unoccupied molecular orbitals (LUMO) and the HOMO-LUMO band gaps for first and second frontier orbitals have been also examined by means of DFT.

Keywords: Density Functional Theory, Electric Dipole Moment, Quadratic Hyperpolarizability, HOMO-LUMO Energies, Nonlinear Optics