P 7. THEORETICAL INVESTIGATIONS ON STATIC FIRST HYPERPOLARIZABILITIES OF N,N'-DIBENZYLIDENE-4-BROMOBENZENE-1,2-DIAMINE

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ABSTRACT: To investigate second-order nonlinear optical (NLO) phenomena of N,N'-dibenzylidene-4-bromobenzene-1,2-diamine, the electric dipole moment and static second-order hyperpolarizability values have been calculated by means of Finite Field (FF) procedure. The basic structure of the title material is based on the π-bond system, due to the overlap of π-orbital delocalization of electronic charge distribution leads to a high mobility of the electron density. The computation results with non-zero values on first hyperpolarizability indicate that the examined compound might possess microscopic second-order NLO behaviour.

Keywords: Second-order Optical Nonlinearity, Electric Dipole Moment, Finite Field, π-bond system, First Hyperpolarizability.