

**P 5. DETERMINATION OF LINEAR AND NONLINEAR OPTICAL BEHAVIOUR OF  
NOVEL TETRAAZAMACROCYCLE DERIVATIVES**

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**ABSTRACT:** In this study; the electric dipole moments, static first and hyperpolarizabilities, dynamic linear polarizabilities, first and second hyperpolarizabilities of the title tetraazamacrocycle compounds, (6E,8E,15E,17E)-7,16-bis(3,3-dimethyl-3H-indol-2-yl)-2,3,11,12-tetrakis(octyloxy)-5,14-dihydrodibenzo[b,i][1,4,8,11]tetraazacyclotetradecine (**1**) and (6E,8E,15E,17E)-7,16-bis(3,3-dimethyl-3H-pyrrolo[3,2-h]quinolin-2-yl)-2,3,11,12-tetrakis(octyloxy)-5,14-dihydrodibenzo[b,i][1,4,8,11]tetraazacyclotetradecine (**2**), have been calculated using ab-initio and density functional theory (DFT) methods. The measured one-photon absorption wavelengths for **1** and **2** are consistence with the theoretically obtained values using time-dependent Hartree-Fock (TDHF) technique. The nonlinear optical results computed here have been compared with the experimental data previously reported in the literature.

*Keywords: Electric Dipole Moment, First Hyperpolarizability, Second Hyperpolarizability, Ab-Initio, Time-Dependent Hartree-Fock*