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Abstract

Synthesis and Nonlinear Optical Studies of N-Containing Heterocyclic Compounds †

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Introduction: The organic compounds which contain a "push–pull" system, that means a couple donor (D)–acceptor (A) connected to a system which contributes to the delocalization of the π-electrons, define the classic structures with optical response due to large hyperpolarizabilities. These arise from a combination of strong electron donor groups (e.g., $–NR_2$, –OR) and strong electron withdrawing groups (e.g., $–NO_2$, –CN), positioned at opposite ends of a conjugated system [1,2] (Figure 1).

Figure 1. Scheme of one organic compound with a "push–pull" system.

Materials and methods: Organic commercial and synthetic materials were used for the synthesis of the heterocyclic compounds. All compounds were characterized with physicochemical techniques (elemental analysis, ^1H, ^{13}C, FTIR, and UV-Vis spectroscopy). The SHG capability of samples was measured by using an experimental set-up [1,3].

Results: A series of N-containing heterocyclic compounds (benzimidazoles, benzothiazole pyrazolones, octahydroacridines) was synthesized and characterized [4–9]. The SHG (second harmonic generation) value was determined for each compound. The molecular polarizability (α), first order hyperpolarizabilities (β_{tot}), dipole (μ_{tot}), and quadrupole (Q) moments, were calculated using DFT (density functional theory) method.

Conclusions: Our results highlight that the nonlinear optical (NLO) response of such small, twisted or flat molecules, mainly depends on the dihedral angles of aromatic and heteroaromatic rings toward the transmitter group. We also found that the electronical and structural peculiarities, of these compounds to be favorable for ultra-fast response times, i.e., femto seconds applications, as confirmed by our previous publications [2,5].

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