Abstract

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

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† Presented at the 17th International Symposium “Priorities of Chemistry for a Sustainable Development” PRIOCHEM, Bucharest, Romania, 27–29 October 2021.

Keywords: organic synthesis; heterocycles; nonlinear optical properties; hyperpolarizability (β)

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., –NR₂, –OR) and strong electron withdrawing groups (e.g., –NO₂, –CN), positioned at opposite ends of a conjugated system [1,2] (Figure 1).

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, 13C, 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 (β̂₁tot), dipole (μ̂tot), 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].

visualization, L.-O.C.; supervision, M.M.; project administration, L.-O.C.; funding acquisition, M.M. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by a grant of the Ministry of Research, Innovation and Digitization CCCDI—UEFISCDI, project number PN-III-P2-2.1-PED-2019-3009, within PNCDI III.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Informed consent was obtained from all subjects involved in the study.

Data Availability Statement: Not applicable.

Acknowledgments: The authors thank the Faculty of Chemistry for the necessary resources provided.

Conflicts of Interest: The authors declare no conflict of interest.

References


