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Abstract

Synthesis, Characterization, DFT Studies, and NLO Properties of Some Benzimidazole Compounds †

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During the last decades, nonlinear optical (NLO) materials have played a significant role because of their various applications in medicine, molecular switches, luminescent materials, laser technology, spectroscopic and electrochemical sensors, data storage, microfabrication and imaging, modulation of optical signals, and telecommunication [1–3]. Organic materials are distinguished by the fact that they exhibit strong NLO properties [2–4]. Recent literature highlights the increased interest in organic materials in recent decades, as an alternative to their inorganic counterparts, and having several advantages, such as their low cost, low toxicity, ease of solution processability, flexibility for device fabrications [5], and modulation of their optical, electronic, and chemical properties by adapting their molecular structure. Organic commercial and synthetic materials were used for the synthesis of the compounds of interest. The second harmonic generation (SHG) capability of samples was measured by using a homemade experimental set-up. A series of benzimidazoles, potential candidates for NLO response, was synthesized. Compounds were characterized by elemental analysis, proton nuclear magnetic resonance spectra(^{1}H-NMR), mass spectra (MS), and Fourrier transform infrared (FTIR) spectra. The analysis of molecular structure and natural bond orbitals (NBOs) was performed using the GAMESS 2012 software. The molecular polarizability α, first-order hyperpolarizabilities β_{tot}, dipole μ_{tot}, and quadrupole (Q) moments were calculated. Our results show that the NLO response of such small, twisted molecules mainly depends on the dihedral angles of aromatic and heteroaromatic rings toward the transmitter group. We expect the structural parameters of these compounds to be favorable for ultrafast response times (i.e., femtoseconds applications). Benzimidazoles are organic compounds suitable for NLO applications, with several advantages: they are cheap and possess low toxicity and ease of solution processability. Density functional theory (DFT) calculations are very useful for the correlation between the NLO behavior of the compounds and their structure for the synthesis of new compounds with improved NLO properties.

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