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Investigations substituent effect on structural, spectral and optical properties of phenylboronic acids

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ABSTRACT

Ortho- and para-substituent arylboronic acid are investigated. Geometric structure and structural properties of these compounds are done. IR and NMR spectrum are calculated for the spectral characterizations. Contour diagram of frontier molecular orbitals which are HOMO and LUMO is calculated and molecular electrostatic potential (MEP) map of them are obtained to evaluate the electronic properties and to determine the active site on the molecules. Non-linear optical (NLO) properties are investigated. UV–VIS spectrum of studied compounds is calculated and the wavelength of main band is examined. Then, some quantum chemical parameters which are total static dipole moment, the average linear polarizability, the anisotropy of the polarizability and first hyperpolarizability are calculated and it was found that B3 is the best NLO material for applications.

1. Introduction

Arylboronic acids are significant compound group due to the fact that they have broad application areas. Although these compounds have been known over more than a hundred years, their properties and application areas are still expanding even today. The most known significant areas are the synthesis of biaryl compounds, molecular receptor, organic framework especially covalent and bioactivity of them [1-8]. The substituent and its location on the phenyl ring are gained significant effect on the acidity, receptor activity, and biological activity, etc. The other important research area is optic. It is known that optical properties of boron compounds have been investigated in many published article [9-14]. In this study, some phenylboronic acids are investigated which their structures are represented in Scheme 1. Ortho- and para- isomers are examined in detail. The whole investigations are performed by molecular simulation analyses. Ortho-substituent aryboronic acid are synthesized by Adamczyk-Wozniak and Sporzynski in 2020 [1].

The goal of this study is the investigating of the structural, spectral and non-linear optical (NLO) properties of mentioned compounds. All these compounds are optimized at M06–2X/6–311G(d) level in gas phase. Structural properties such as bond length, bond angle and geometry are revealed. Structural differences respect to location of substituent are reported in detail. IR and NMR spectrum are calculated for the spectral characterization of studied compounds. Vibration mode of selected peaks are analyzed with utilities. In NMR analyses, chemical shift values of carbon, hydrogen and boron atoms are reported. Molecular orbital energy diagram (MOED), contour plot of frontier molecular orbitals and molecular electrostatic potential (MEP) maps are examined to analyze the electronic properties. Finally, NLO properties are examined by using some parameters and UV–VIS spectrum. Urea is taken into consideration as reference material for the evaluating of the NLO properties of mentioned compounds.

2. Method

Computational analyses of selected phenylboronic acids were performed by licenced softwares. GaussView 6.0.16, Gaussian16 IA32W-G16RevB.01, Gaussian09 AS64L-G09RevD.01, ChemDraw Professional 15.1 and VEDA 4XX programs were used in this project [15-18]. Selected compounds were drawn by using GaussView and pre-optimizations were done by using Gaussian16 IA32W-G16RevB.01 at personal computer. Then, fully-optimizations were performed by using Gaussian09 AS64L-G09RevD.01 program at TR-Grid workstations. Universal force field (UFF) method was used in pre-optimizations while M06–2X/6–311G(d) level in gas phase. IR spectrum of studied phenylboronic acids were analyzed by VEDA 4XX program. gage-Independent Atomic Orbital (GIAO) method was used in the NMR calculations. As for the UV–VIS calculations, time-dependent (TD) method was used in the calculations. The total static dipole moment (μ), the average linear polarizability (α), the anisotropy of the polarizability ($\Delta\alpha$) and first hyperpolarizability (β) are calculated by using the Eq. (1) - (4):

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