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Investigations over Optical Properties of Boron Complexes of Benzothiazolines

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Abstract: Quantum chemical analyses over benzothiazolines and their boron complexes are performed. In calculations, M06-2X method was selected with 6-31+G(d,p) level. Structural and spectral (IR and NMR) characterization of studied compounds are done in detail. Quantum chemical descriptors (QCDs) are calculated to investigate the optical properties. Furthermore, molecular electrostatic potential (MEP) maps of the studied compounds are calculated by using electro-static potential (ESP) charges. According to QCDs and MEP maps, NLO properties of boron complexes are more than those of benzothiazolines and (Z)-2-((pyridin-2-ylmethylene)amino) benzenethiolatebutane-1,3-bis(olate)boron(III), complex **(7)**, has the most NLO activity in studied compounds. Finally, solvent effect on NLO activity are investigated by calculating UV-VIS spectrum in gas phase (ε=1), toluene (ε=2.3741), chloroform (ε=4.7113), methanol (ε=32.613), water (ε=78.3553) and n-methylformamide-mixture (ε=181.56). According to these spectra results, NLO activity mainly increases with increasing of polarizability of media.

Keywords: Benzothiazoline, Boron Complexes, Molecular Simulation, DFT Studies, NLO Properties

1. Introduction

Benzothiazoline is known as member of class of heteroaromatic and composed of benzene-fused protonated thiazole ring at the ring nitrogen [1]. Benzothiazoline has broad applications in biological and medicinal activities [2-5]. Although benzoxazolines have been studied many time, benzothiazolines have been studied less. In many literatures, biological and medicinal importance of this class have been highlighted many times. Boron and its compounds have optical and medicinal properties [6-10]. Boron and its compounds have been popular recent years due to the broad application areas. 2-(thiophen-2-yl)-2,3-dihydro-1,3-benzothiazole, 2-(furan-2-yl)-2,3-dihydro-1,3-benzothiazole, 2-(pyridin-2-yl)-2,3-dihydro-1,3-benzothiazole and their boron complexes have been synthesized by Pandey and Singh in 2000 [11]. Their optical properties have not investigated yet. Additionally, their structural properties have not reported yet. In this study, 2-phenyl-2,3-dihydrobenzothiazoline **(1)**, 2-(pyridin-2-yl)-2,3-dihydrobenzothiazoline **(2)** 2-(thiophen-2-yl)-2,3-dihydro-1,3-benzothiazoline **(3)**, 2-(furan-2-yl)-2,3-dihydro-1,3-benzothiazoline **(4)**, (Z)-2-(benzylideneamino)benzenethiolatebutane-1,3-bis(olate)boron(III) **(5)**, (Z)-2-(benzylideneamino)benzenethiolatepropane-1,2-bis(olate)boron(III) **(6)**, (Z)-2-((pyridin-2-ylmethylene)amino) benzenethiolatebutane-1,3-bis(olate)boron(III) **(7)**, (Z)-2-((pyridin-2-ylmethylene)amino)benzenethiolate propane-1,2-bis(olate)boron(III) **(8)**, (Z)-2-((thiophen-2-ylmethylene)amino)benzenethiolatebutane-1,3-bis(olate)boron(III) **(9)**, (Z)-2-((thiophen-2-ylmethylene)amino)benzenethiolatepropane-1,2-bis(olate)boron(III) **(10)**, (Z)-2-((furan-2-ylmethylene)amino)benzenethiolatebutane-1,3-bis(olate)boron(III) **(11)** and (Z)-2-((furan-2-ylmethylene)amino)benzenethiolatepropane-1,2-bis(olate)boron(III) **(12)** are investigated in detail. The simple structure of them are represented in Scheme 1.