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Quantum mechanical study of Derivative of Thiadiazole and Quinoxaline molecules using density functional theory

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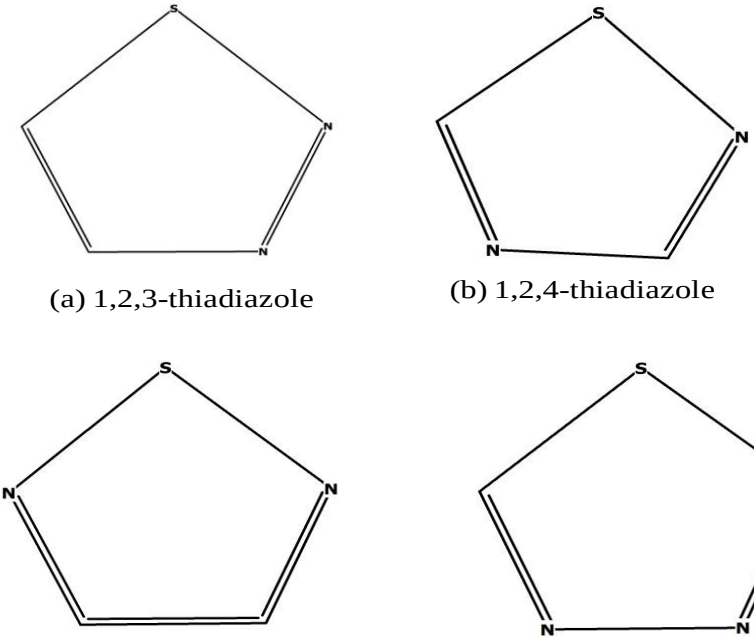
Abstract: Thiadiazole Derivatives are widely employed in the fields of pharmaceutical, agricultural, industrial and polymer chemistry. The electronic and molecular structures of thiadiazoles are of interest because they have similar numbers of valence electrons and similar molecular structures to thiophenes, which are currently used in the manufacture of organic solar cells due to their relatively high hole mobility and good light harvesting properties. For this reason, the electronic properties of 1,3,4-thiadiazole derivatives warrant investigation. In the present work, we investigated IR activity and thermodynamical properties of derivative of thiadiazole.

All calculations were performed by applying the B3LYP/6-311G chemical model in the Gaussian 09W and GaussView software packages.

Keywords: Thiadiazole Derivatives, vibrational spectrum, DFT

INTRODUCTION

Due to the aging and growth of the population, the number of new cancer cases is expected to increase. Although substantial progress had been made in the understanding of the molecular biology of particular cancer types, and many potentially specific therapeutic targets were identified in recent years, the development of better anticancer therapeutic strategies is needed.



(a) 1,2,3-thiadiazole (b) 1,2,4-thiadiazole

(c) 1,2,5-thiadiazole (d) 1,3,4-thiadiazole

Figure 1:- Core structures of the thiadiazole isoforms occurring in nature.

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Thiadiazole is a five-membered heterocyclic compound containing one sulfur and two nitrogen atoms. It occurs in nature in four isoforms: 1,2,3-thiadiazole, 1,2,4-thiadizaole, 1,2,5-thiadiazole and 1,3,4-thiadiazole (Fig. 1). Taking into account that thiadiazole is the bioisostere of pyrimidine and oxadiazole, it is not surprising that compounds bearing this moiety present a broad spectrum of pharmacological properties, including antiviral, antibacterial, antifungal, antiparasitic, anti-inflammatory and anticancer activities [1-6]. Due to the mesoionic nature, thiadiazoles are able to cross the cellular membranes. Their relatively good liposolubility is most likely attributed to the presence of the sulphur atom [6-10]. The thiadiazole-containing drugs, including diuretics acetazolamide and methazolamide or antibiotics cefazedone and cefazolin sodium, are already used in clinics. Accumulating evidence has also revealed several thiadiazole derivatives that exhibit anticancer activities in various in vitro and in vivo models. In addition, several thiadiazole-containing compounds have gone into clinical trials as a single agent or in combination with existing anticancer drugs [10-12].

One of the first studies documenting the anti-cancer activity of 1,3,4-thiadiazole derivatives was published in 1957 by Shapiro et al.. In this paper, 2-ethylamino 1,3,4-thiadiazole (EATDA), an analog of niacin, inhibits the growth of induced mammary adenocarcinoma in rats. The anti-tumor effect of this compound was prevented by pre-injection of nicotinamide. Supporting evidence that it is a niacin antagonist. In addition, the addition of EATDA to the combination of 8-azaguanine, deoxypyridoxine and testosterone improved the anticancer activity of this three-drug combination [4]. In addition, they were found to be useful in treatment of respiratory diseases, cardiovascular diseases, tumors, hemorrhage, sepsis, and fever [12-18]. In view of these facts, we have taken some thiadiazoles based on 1,3,4-thiadiazole moiety with anticipated biological properties.

COMPUTATIONAL METHODOLOGY

In The present work, we carried out DFT calculations along with B3LYP/6-311G level of theory using Gaussian 09 pakage. Derivative of Thiadiazole and Quinoxaline molecules were built and viewed through Gaussview visualize [19-25]. Vibrational and thermodynamical parameters were determined by following optimization and frequency calculations.

RESULTS AND DISCUSSION

Optimized geometries of Derivative of Thiadiazole and Quinoxaline molecules are shown in Fig.2 and minimum energy values of molecules are -2294.07 a.u. ,-2441.61 a.u. & -1871.18 a.u. respectively. Quantum mechanical DFT analysis revealed that all derivatives have lowest energy and stable geometry.

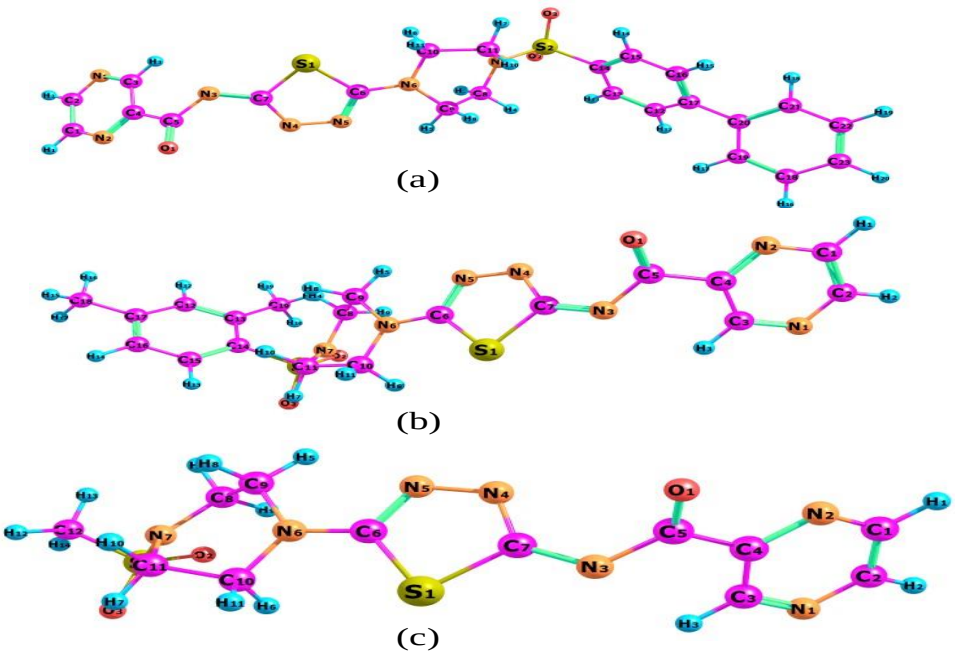

Figure 2:- Optimized geometries of Derivative of Thiadiazole and Quinoxaline molecules

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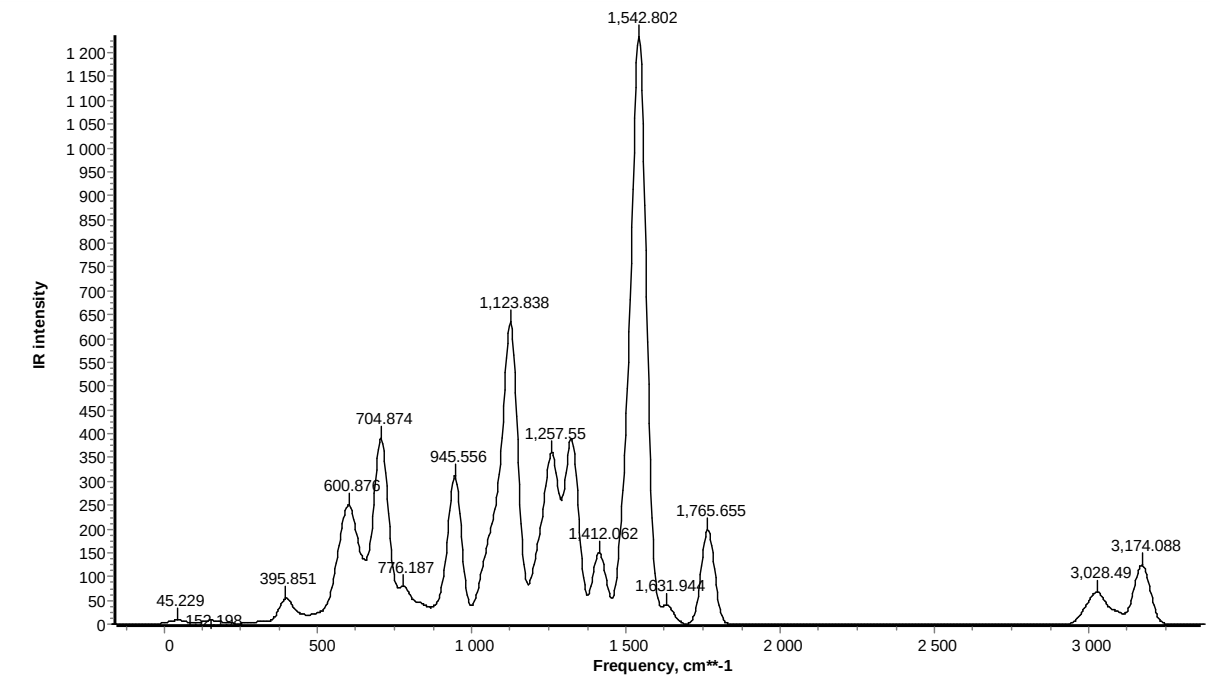
Thermodynamic parameters of Derivative of Thiadiazole and Quinoxaline molecules in the stable states are shown in the table 1. IR activity of the molecules is the analysis of IR light with molecules. This is analyzed by three ways such as reflection, emission and absorption. IR Spectroscopy measures the vibrations of atoms, and based on this it is possible to determine the functional groups. Generally, stronger bonds and light atoms will vibrate at a high stretching frequency. The IR activity of the Derivative of Thiadiazole and Quinoxaline molecules are shown in the Fig. 3 (a), (b) and (c) respectively.

Table 1:- Thermodynamic parameters of Derivative of Thiadiazole and Quinoxaline molecules

Molecules	Thermal energy ($E_{thermal}$) Kcal/mol	Specific heat constant (C_v) Cal/mol-K	Entropy (S) Cal/mol-K
TD1	277.066	114.122	209.972
TD2	260.216	106.881	201.664
TD3	188.386	81.538	168.021



(a)

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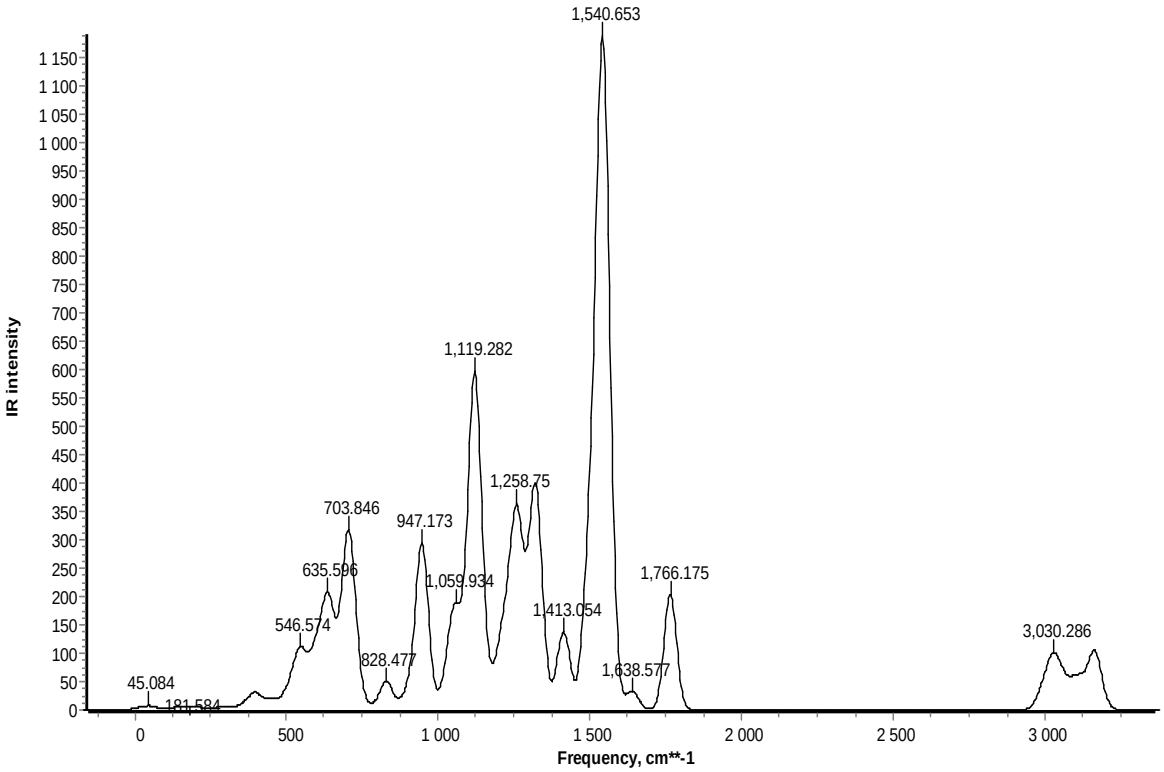
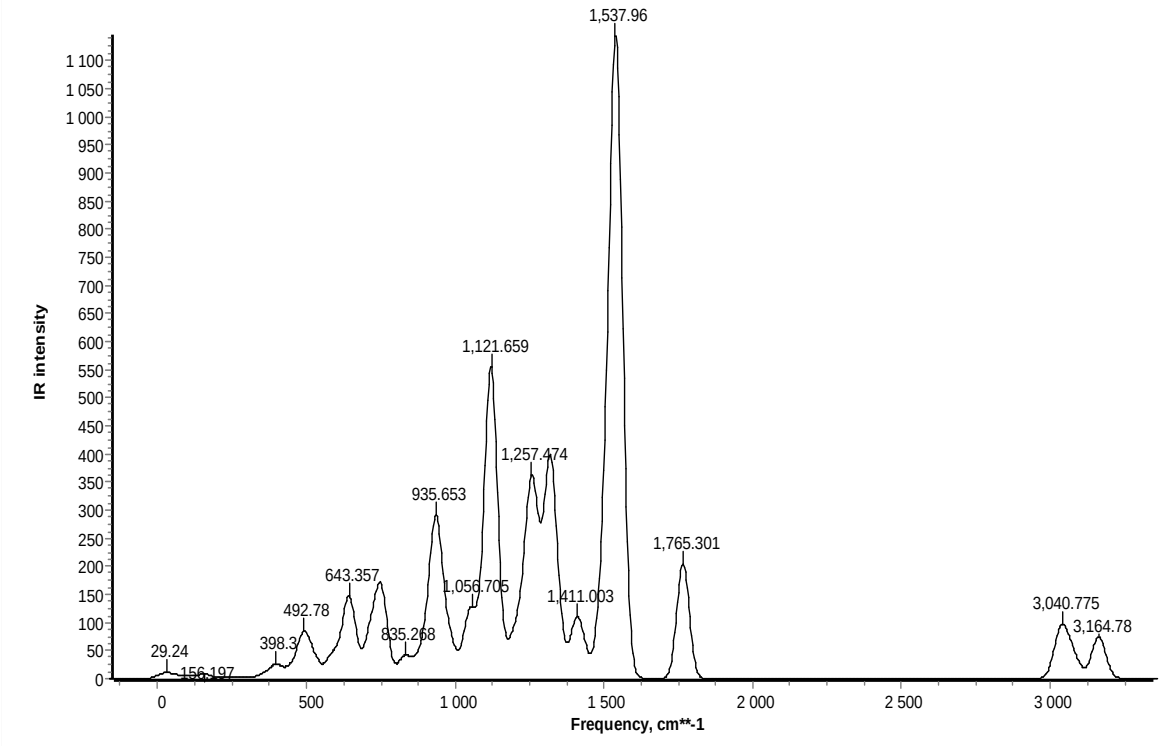


(b)



(c)

Figure 3:- IR activity of Derivative of Thiadiazole and Quinoxaline molecules

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The aromatic C-H stretching occurs above 3000 cm^{-1} and is typically exhibited as a multiplicity of weak to moderate bands. The bands are weak due to decrease of dipole moment caused by the reduction of negative charge on carbon atom. Stretching in C=N at frequency 1542.80 cm^{-1}, 1540.65 cm^{-1} and 1537.96 cm^{-1} respectively.

CONCLUSION

In this theoretical study, various thiadiazole derivatives were analyzed through the application of vibrational and thermodynamical theory and investigated IR, thermal energy, specific heat capacity and Entropy. From the results it is noticed that the peak of IR changed due to the length of molecules. Frequency at which stretching the C=N bond are displaced due to the length of molecules.

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