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Ab initio studies on optimized geometries for the thiazole derivatives

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ABSTRACT

The molecular geometry and energies of N,N'-bis(2-Thiazol-yl)methylenediamin (1) in the ground state are calculated by using the HF method with 6-31G basis sets. The calculated HOMO and LUMO energies also confirm that charge transfer occurs within the molecule. The geometries and energies obtained from HF/6-31G* calculations are in good agreement with the experimentally observed data.*

Keywords: N,N'-bis(2-Thiazol-yl)methylenediamin, HF, HOMO, LOMO.

INTRODUCTION

2-Aminothiazole derivatives are widely used as pharmaceuticals. For example, Talipexol [1] and Pramipexole [2] with a 2-aminothiazole moiety are used as antiparkinsonian drugs and dopamine agonists; Tigemonam [3] is an antibacterial drug and Amthamine [4] is known as an antiasthmatic one. It is also known that heterocyclic compounds with free amino groups may exhibit teratogenic and mutagenic properties because of their ability to form non-covalent complexes with DNA [5,6]. That is why 2-aminothiazole derivatives with an acylated amino group may be of interest as potentially less toxic drugs with a wide variety of pharmacological activities. A number of publications have described the synthesis of 2-aminothiazoles, N-acylated with aliphatic [7-11], aromatic [7,8,10], dicarboxylic acids [10,12-16] and azo substituent [17]. The importance of such derivatives is due to their biological properties; for example, some of them show significant bacteriostatic [7], tuberculostatic [8], hypoglycemic, anti-inflammatory, diuretic and fungicidal activities [10], and some of them are useful for treating of asthma [14]. Derivatives of thiazole have anti-inflammatory activity [18] antituberculosis [19], antioxidant activity [20] and antibacterial [21] properties.

In this study, molecular geometry, optimized parameters and energies are computed and the performance of the computational methods for ab initio level at 6-31G* basis sets are compared.

The HOMO represents the ability to donate an electron, LUMO as an electron acceptor represents the ability to obtain an electron the HOMO and LUMO energy calculated by HF at 6-31G* method.

Computational Details

All calculations were performed using the Gaussian 98 package of program [22] on a Windows-XP operating PC. The molecular structure of the title compound in the ground state is computed by performing both HF with 6-31G* basis set.

RESULTS AND DISCUSSION

The optimized molecular structure of title molecule is obtained from Gaussian 98 and GaussView 3.0 programs are shown in the Figure 1.

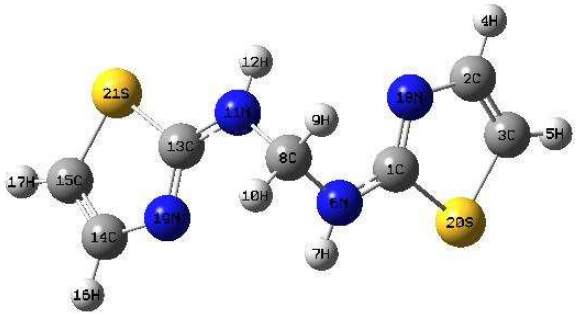

Fig. 1. Numbering system adopted in the study for (1) by using HF/6-31G*

Computational (theoretical) calculations energy differences for the compound (1) were determined by optimizing the geometry at various computational levels. Comparison of the energies at the HF/6-31G* level listed in Table 1 shows the differences in the energies.

Table 1. Theoretically computed energies (a.u.), zero-point vibrational energies (kcal mol^{-1}), rotational constants (GHz), entropies (cal mol^{-1} K^{-1}) for compound of (1) at the HF/6-31G*

Parameters	HF(6-31G*)
Total energy	-1282.2396
Zero-point energy	104.9705
Rotational constants	1.4567
	0.2873
	0.2777
Entropy total	103.982
Translational	41.958
Rotational	32.292
Vibrational	34.732

The optimized structural parameters of compound (1) calculated by ab initio-HF level with the standard 6-31G* basis set are listed in Table 2.

Table 2. Geometrical parameters optimized of compound (1), bond length (Å) and angle (°) at the HF/6-31G*

Bond lengths	HF 6-31G*	Bond length	HF 6-31G*
C(1)-N(18)	1.290	N(19)-C(13)-S(21)	114.00
C(1)-S(20)	1.811	N(19)-C(13)-N(11)	124.42
C(1)-N(6)	1.348	S(21)-C(13)-N(11)	121.56
N(18)-C(2)	1.395	C(13)-N(19)-C(14)	112.49
S(20)-C(3)	1.809	C(13)-S(21)-C(15)	86.95
C(2)-C(3)	1.336	N(19)-C(14)-C(15)	116.77
N(6)-C(8)	1.448	S(21)-C(15)-C(14)	109.76
C(8)-N(11)	1.448	N(11)-C(8)-N(6)	113.76
N(11)-C(13)	1.348	N(6)-C(1)-S(20)	121.57
C(13)-N(19)	1.290	N(6)-C(1)-N(18)	124.41
C(13)-S(21)	1.811	S(20)-C(1)-N(18)	112.49
N(19)-C(14)	1.395	C(1)-N(18)-C(2)	114.00
S(21)-C(15)	1.809	C(1)-S(20)-C(3)	86.95
C(14)-C(15)	1.336	N(18)-C(2)-C(3)	116.77
		S(20)-C(3)-C(2)	109.76

The HOMO represents the ability to donate an electron, LUMO as an electron acceptor represents the ability to obtain an electron the HOMO and LUMO energy calculated by HF level with the 6-31G* basis set Figure 2. This electronic absorption corresponds to the transition from the ground to the first excited state and is mainly described by one electron excitation from the highest occupied molecular or orbital (LUMO).

E_{LUMO} = 0.08419 a.u E_{HOMO} = -0.41822 a.u

ΔE = 0.50241 a.u

Fig. 2. The atomic orbital compositions of the frontier molecular orbital for compound (1) by using HF/6-31G*

The HOMO is located over the group, the HOMO→LUMO transition implies an electron density transfer to ring from chlorine and partially from ring.

CONCLUSION

Ab initio level at 6-31G* basis sets calculations were carried out on N,N'-bis(2-Thiazol-yl)methylenediamin. The HF method with the 6-31G* basis set have been used to determine the ground state geometries, energies of compound (1).

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