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Theoretical Study of Reactivity and Stability of a Thiazine Derivative Series by the Density Functional Theory (DFT) Method

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Abstract The study of the reactivity and stability of the five (05) compounds of Thiazine was carried out using the density functional theory at the level B3LYP/6-31+ G (d, p). The determination of the dual descriptor as well as the analysis of the map of the molecular electrostatic potential (MEP) made it possible to show that the sulfur and nitrogen atoms of the Thiazine cycle are respectively the electrophilic and nucleophilic sites. The study of the chemical reactivity of our compounds was carried out from the analysis of the frontier molecular orbitals (HOMO and LUMO), the energy gap (ΔE), the chemical hardness (η), the electrophilicity index (ω) and electronegativity (χ). Thus, the Thz3 compound is the least reactive, the least electron donor and the most stable of all our compounds.

Keywords: *Thiazine, DFT, MEP, reactivity, stability*

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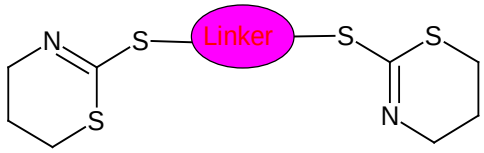
1. Introduction

Heterocycles are defined as chemical species whose carbon chain contains one or more carbon atoms are substituted by heteroatoms such as nitrogen, sulfur, oxygen, phosphorus, etc. [1,2]. Heterocycles possess structural variety and are used in several fields. Heterocyclic compounds comprising nitrogen and sulfur atoms are widely used in coordination chemistry for the development of new bioactive molecules [3,4,5]. In the case of our study, we are interested in Thiazine derivatives which are six-membered ring systems containing endocyclic sulfur and nitrogen atoms [6]. In addition to their biological activity, Thiazines are used in the dye and insecticide industries [7]. Nowadays one of the methods allowing to give a lot of information on the molecular electronic structures and contributes to the evolution experimental chemistry is the computational chemistry [8,9], thus, it makes it possible to reduce the number of experiments, often long, dangerous and costly in time and money [10,11]. The stability is a theoretical study that predicts the global and local reactivity sites of a molecule [12]. The general objective of this work is to theoretically determine the reactivity, to identify the nucleophilic/electrophilic attack sites by different methods of quantum chemistry.

Table 1. Structures of the studied Thiazine derivatives



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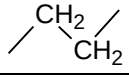
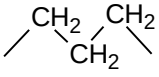
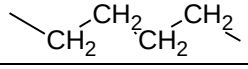
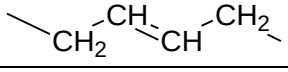
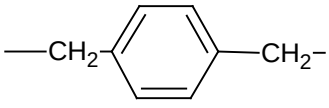
Thz1	
Thz2	
Thz3	
Thz4	
Thz5	

2. Materials and Methods

2.1. Computational Theory Level

The theoretical study of chemical reactivity has been conducted based on three theoretical approaches. The first one concerns the analysis of electrostatic potential maps. The second approach is concerned with the local indices of reactivity and the dual descriptors. The last approach is related to the boundary molecular orbitals. The geometries of the molecules have been optimized at the DFT level with the B3LYP [13,14] in the 6-31+G(d,p) basis using the Gaussian 09 software [15]. This Hybrid functional gives better energies and is in agreement with high level ab initio methods [16,17]. The geometries are held constant for both cationic and anionic systems. The global reactivity indices were obtained from the conceptual DFT model [18,19].

2.2. Reactivity Descriptors

2.2.1. Electrostatic Potential Surface Area

The analysis of the surface of the electrostatic potential makes it possible to highlight the zones capable of being nucleophilic or electrophilic attack sites. The analysis of this surface is based on the colors. The potential increases in the order red < orange < yellow < green < cyan < blue [20,21]. In the electrostatic potential surface, areas that have zero potential are represented by the color green, negative areas (red and yellow) are electrophilic attack sites, and positive areas (cyan and blue) are electrophilic attack sites. nucleophilic attack.

2.2.2. Global Descriptors

To predict the chemical reactivity, some theoretical descriptors related to the conceptual DFT have been determined. In particular, the energy of the lowest vacant molecular orbital (MO) ($\mathbf{E_{LUMO}}$), the energy of the highest occupied molecular orbital (MO) ($\mathbf{E_{HOMO}}$), the electronegativity (χ), the global softness (σ) and the global electrophilicity index (ω). These descriptors are all determined from the optimized molecules. It should be noted that, the descriptors related to the boundary molecular orbitals were calculated in a very simple way within the Koopmans approximation [22]. The LUMO energy characterizes the sensitivity of the molecule to a nucleophilic attack, and as for the HOMO energy, it characterizes the susceptibility of a molecule to an electrophilic attack. The electronegativity(χ) is the parameter which translates the aptitude of a molecule not to let escape its electrons. The overall softness (σ) expresses the resistance of a system to the change of its number of electrons. The global electrophilicity index characterizes the electrophilic power of the molecule. These different parameters are calculated from equations (1-6):

$$I = -E_{HOMO} \tag{1}$$

$$A = -E_{LUMO} \tag{2}$$

$$\chi = -\mu = -1/2\left(E_{LUMO} + E_{HOMO}\right) \tag{3}$$

$$\eta = \left(E_{LUMO} - E_{HOMO}\right)/2 \tag{4}$$

$$\omega = \frac{\chi^2}{2\eta} \tag{5}$$

$$\sigma = 1/\eta \tag{6}$$

2.2.3. Local and Dual Descriptors

The Fukui numbers of a molecule give information about the local reactivity in a molecule. The atom with the largest Fukui number is more reactive than the other atoms in the molecule [23]. These indices represent the qualitative description of the reactivity of atoms in the molecule. The Fukui function successfully predicts the relative reactivity for most chemical systems. The determination of Fukui indices for the selectivity of electrophilic and nucleophilic atoms in chalcone-derived compounds has been done. Ayers and Parr [24]. Explained that molecules tend to react where the Fukui function is largest when attacked by soft reagents and in places where the Fukui function is smallest when attacked by hard reagents. Using the Natural Atomic Population charges of the optimized ground state compounds, the Fukui function (f_k^+, f_k^-), local softness (s_k^+, s_k^-) and local indices of electrophilia (ω_k^+, ω_k^-) [25], have been determined. The Fukui functions are calculated using equations (7) and (8):

$$f_k^+ = q_k\left(N+1\right) - q_k\left(N\right) \tag{7}$$

$$f_k^- = q_k\left(N\right) - q_k\left(N-1\right) \tag{8}$$

f_k^+ for nucleophilic attack

f_k^- for electrophilic attack

$q_k\left(N\right)$: Electronic population of atom k in the neutral molecule.

$q_k\left(N+1\right)$: Electronic population of atom k in the anionic molecule.

$q_k\left(N-1\right)$: Electronic population of atom k in the cationic molecule.

The values of the dual descriptors [26] are obtained from equation (9)

$$\Delta f = f_k^+ - f_k^-. \tag{9}$$

2.3. Natural Population Analysis (NPA)

The calculation of natural atomic charge plays an important role in the study of molecular systems in quantum chemistry. For the quantitative description of a molecular charge distribution, the molecule is dissected into well-defined atomic fragments. A general and natural choice is to share the charge density at each point between the different atoms in proportion to their free atom densities at the corresponding distances of the nuclei [1]. In this work, the atomic charge values were obtained by the Natural population analysis.

3. Results and Discussion

3.1. Local Reactivity

3.1.1. Electrostatic Potential Surface

In order to have a general idea about the sites of reactivity of the compounds, we analyzed the potential energy surface of each of these compounds. Images of these maps are shown in Figure 1.

The surface of electrostatic potential, areas that have zero potential are represented by the color green, negative areas (red and yellow) are electrophilic etch sites, and positive areas (cyan and blue) are etch sites nucleophiles. The analysis of these maps indicates that the sulfur atoms (s) are the sites of electrophilic attacks because a neighborhood of negative potential is observed around these atoms. As for nucleophilic attack sites in this study, nitrogen atoms are the most available.

3.1.2. Determination of Dual Descriptors

The determination of the dual descriptor allows us to locate the nucleophilic and electrophilic sites of the five (05) compounds derived from Thiazines. In this study we calculated the Fukui indices (f+, f-) and the dual descriptor (Δf(r)) and the results shown in Table 2 to Table 6.

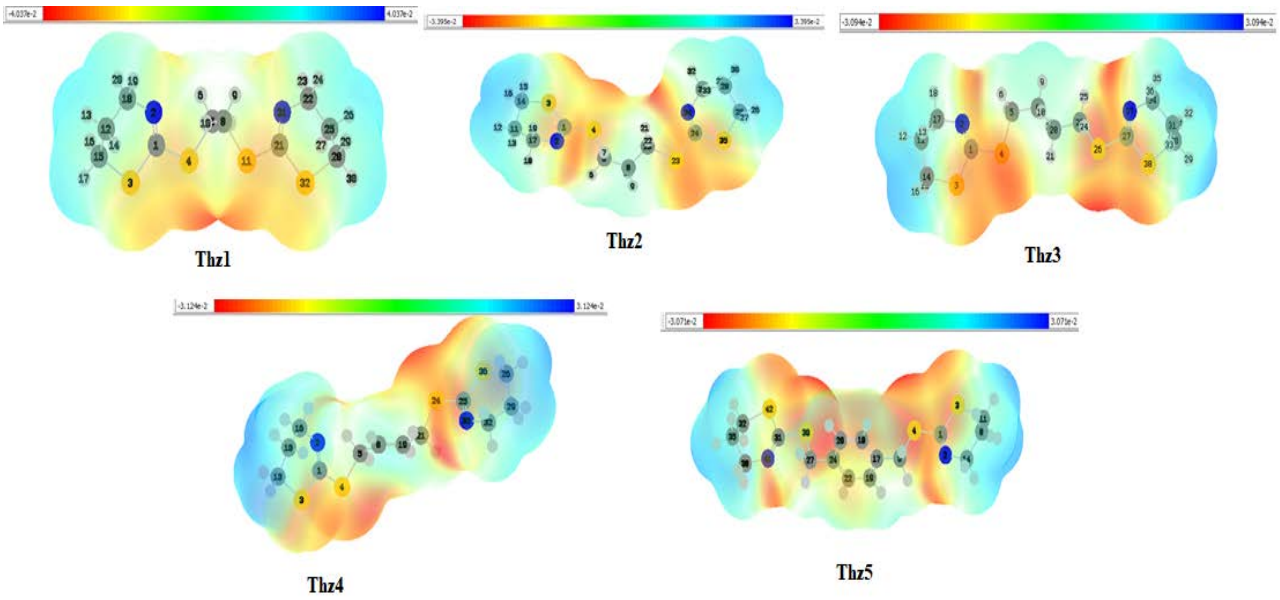
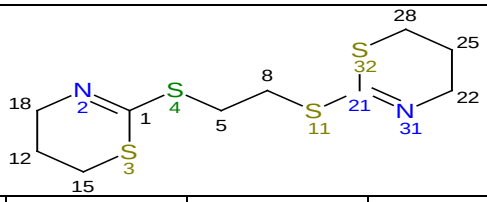


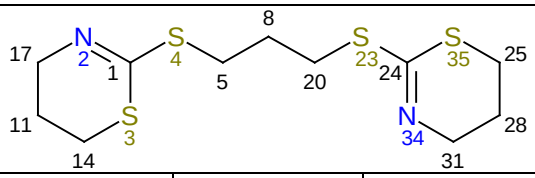
Figure 1. Molecular Electrostatic Potential (MEP) surface of compounds Thz1 to Thz5

Table 2. Local reactivity descriptors of compound Thz1 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d, p) level



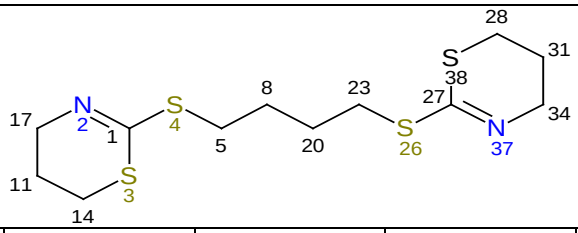
Atomes	Q(N)	Q(N+1)	Q(N-1)	f+	f-	Δf(r)
C1	6.067	5.993	6.232	-0.074	-0.165	0.091
N2	7.533	7.304	7.003	-0.229	0.530	**-0.759**
S3	15.749	15.888	15.875	0.139	-0.126	**0.265**
S4	15.715	15.874	15.478	0.159	0.237	-0.079
C5	6.620	6.293	6.316	-0.327	0.304	-0.632
C8	6.620	6.293	6.316	-0.327	0.304	-0.631
S11	15.715	15.874	15.478	0.159	0.237	-0.079
C12	6.508	6.231	6.239	-0.277	0.269	-0.546
C15	6.609	6.281	6.290	-0.328	0.319	-0.646
C18	6.295	6.113	6.152	-0.181	0.142	-0.324
C21	6.067	5.993	6.232	-0.074	-0.165	0.091
C22	6.295	6.113	6.152	-0.181	0.142	-0.324
C25	6.508	6.231	6.239	-0.277	0.269	-0.546
C28	6.609	6.281	6.290	-0.328	0.319	-0.646
N31	7.533	7.304	7.003	-0.229	0.530	**-0.759**
S32	15.749	15.888	15.875	0.139	-0.126	**0.265**

Table 3. Local reactivity descriptors of compound Thz2 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d, p) level



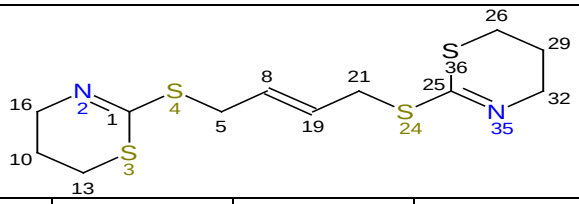
Atomes	Q(N)	Q(N+1)	Q(N-1)	f+	f-	Δf(r)
C1	6.066	6.021	6.056	-0.045	0.010	-0.055
N2	7.522	7.265	7.251	-0.258	0.271	-0.529
S3	15.753	15.880	15.719	0.127	0.034	0.092
S4	15.734	15.871	15.626	0.137	0.108	0.029
C5	6.595	6.292	6.307	-0.302	0.287	-0.589
C8	6.501	6.246	6.255	-0.255	0.246	-0.500
C11	6.508	6.245	6.256	-0.263	0.252	-0.515
C14	6.609	6.288	6.309	-0.321	0.300	-0.621
C17	6.296	6.140	6.152	-0.156	0.144	-0.300
C20	6.603	6.298	6.310	-0.304	0.292	-0.597
S23	15.729	15.873	15.652	0.144	0.077	0.067
C24	6.066	6.023	6.088	-0.043	-0.022	-0.021
C25	6.609	6.288	6.307	-0.320	0.301	-0.622
C28	6.508	6.246	6.256	-0.262	0.252	-0.514
C31	6.296	6.142	6.159	-0.154	0.137	-0.291
N34	7.521	7.260	7.074	-0.261	0.447	**-0.709**
S35	15.754	15.883	15.765	0.129	-0.011	**0.140**

Table 4. Local reactivity descriptors of compound Thz3 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d, p) level



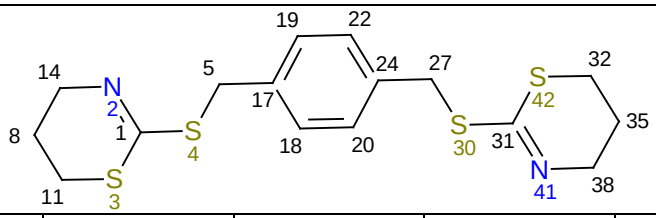
Atomes	**Q(N)**	**Q(N+1)**	**Q(N-1)**	**f+**	**f-**	**Δf(r)**
C1	6.066	6.019	6.056	-0.046	0.009	-0.056
N2	7.522	7.263	7.251	-0.260	0.271	-0.531
S3	15.753	15.881	15.716	0.128	0.038	0.090
S4	15.735	15.874	15.621	0.139	0.115	0.024
C5	6.594	6.294	6.306	-0.301	0.288	-0.589
C8	6.483	6.238	6.245	-0.245	0.237	-0.482
C11	6.508	6.245	6.256	-0.263	0.252	-0.515
C14	6.609	6.289	6.309	-0.320	0.300	-0.620
C17	6.296	6.140	6.152	-0.156	0.144	-0.299
C20	6.493	6.245	6.248	-0.248	0.245	-0.493
C23	6.596	6.295	6.307	-0.301	0.290	-0.591
S26	15.725	15.870	15.669	0.145	0.056	0.089
C27	6.067	6.022	6.087	-0.045	-0.020	-0.025
C28	6.609	6.289	6.308	-0.320	0.302	-0.622
C31	6.508	6.246	6.257	-0.262	0.251	-0.514
C34	6.296	6.141	6.159	-0.155	0.137	-0.293
N37	7.522	7.262	7.074	-0.260	0.449	**-0.709**
S38	15.754	15.882	15.762	0.128	-0.008	**0.136**

Table 5. Local reactivity descriptors of compound Thz4 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d, p) level



Atomes	Q(N)	Q(N+1)	Q(N-1)	f+	f-	Δf(r)
C1	6.065	6.021	6.081	-0.045	-0.016	-0.029
N2	7.530	7.267	7.105	-0.263	0.425	**-0.688**
S3	15.749	15.878	15.805	0.130	-0.056	**0.186**
S4	15.724	15.866	15.641	0.142	0.083	0.059
C5	6.625	6.306	6.324	-0.319	0.301	-0.619
C8	6.214	6.100	6.065	-0.114	0.150	-0.264
C10	6.508	6.247	6.256	-0.261	0.252	-0.513
C13	6.609	6.287	6.306	-0.322	0.302	-0.624
C16	6.295	6.141	6.157	-0.154	0.137	-0.291
C19	6.237	6.116	6.086	-0.121	0.151	-0.272
C21	6.616	6.301	6.316	-0.315	0.300	-0.615
S24	15.728	15.866	15.675	0.138	0.053	0.085
C25	6.067	6.027	6.055	-0.040	0.012	-0.053
C26	6.609	6.288	6.309	-0.321	0.300	-0.621
C29	6.508	6.246	6.255	-0.262	0.254	-0.515
C32	6.296	6.142	6.151	-0.154	0.145	-0.299
N35	7.523	7.265	7.217	-0.257	0.305	-0.563
S36	15.754	15.881	15.715	0.128	0.039	0.089

Table 6. Local reactivity descriptors of compound Thz5 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d. p) level



Atomes	Q(N)	Q(N+1)	Q(N-1)	f+	f-	Δf(r)
C1	6.070	6.020	6.055	-0.050	0.014	-0.064
N2	7.523	7.259	7.239	-0.264	0.284	-0.548
S3	15.753	15.884	15.733	0.131	0.020	0.111
S4	15.720	15.868	15.655	0.148	0.065	0.083
C5	6.595	6.294	6.306	-0.302	0.290	-0.591
C8	6.508	6.247	6.255	-0.262	0.253	-0.514
C11	6.609	6.291	6.309	-0.318	0.300	-0.618
C14	6.296	6.141	6.151	-0.155	0.145	-0.299
C17	6.064	6.037	6.014	-0.028	0.051	-0.079
C18	6.221	6.100	6.074	-0.121	0.147	-0.267
C19	6.221	6.102	6.115	-0.118	0.106	-0.224
C20	6.221	6.100	6.115	-0.121	0.106	-0.227
C22	6.221	6.102	6.073	-0.118	0.148	-0.266
C24	6.064	6.037	6.015	-0.028	0.049	-0.077
C27	6.595	6.294	6.305	-0.302	0.290	-0.592
S30	15.720	15.868	15.690	0.148	0.029	0.119
C31	6.070	6.020	6.080	-0.050	-0.011	-0.039
C32	6.609	6.291	6.306	-0.318	0.303	-0.620
C35	6.508	6.247	6.257	-0.262	0.251	-0.512
C38	6.296	6.141	6.157	-0.155	0.139	-0.294
N41	7.523	7.259	7.092	-0.264	0.431	**-0.695**
S42	15.753	15.884	15.782	0.131	-0.029	**0.160**

The different results obtained from the calculation of the dual descriptor show that the sulfur (S) atoms of the Thiazine nucleus indicate the greatest values of the dual descriptor. which from them the electrophilic sites. As for the Nitrogen (N) atoms of the Thiazine ring. they display the lowest values of the dual descriptor. These low values show that these nitrogen atoms are the nucleophilic sites of the Thiazine derivatives studied.

3.2. Overall Reactivity

The study of the global reactivity of molecules is based on the calculation of global indices deduced from the electronic properties. The values of the energies related to the molecular frontier orbitals are given in Table 7. In view of these values we note the largest value of the energy gap for the compound Thz3 (ΔE= 5.915 eV). which allows us to say that it is less reactive of our compounds. However, the compound Thz5 would be more reactive because it has the smallest value of the energy gap (ΔE= 5.442 eV). of this series studied. Thus. the compounds are classified in the following descending order of stability:

$$\Delta E : Thz3 > Thz2 > Thz1 > Thz4 > Thz5$$

Table 7. Energy descriptors of the studied compounds

Compounds	E_{HOMO}(eV)	E_{LUMO}(eV)	ΔE(eV)	I(eV)	A(eV)
Thz1	-6.342	-0.512	5.830	6.342	0.512
Thz2	-6.323	-0.443	5.880	6.323	0.443
Thz3	-6.328	-0.413	5.915	6.328	0.413
Thz4	-6.339	-0.627	5.712	6.339	0.627
Thz5	-6.342	-0.900	5.442	6.342	0.900

Table 8 shows the overall reactivity indices of the Thiazine derivatives studied.

Table 8. Global descriptors of chemical reactivity of studied compounds

Compounds	χ(eV)	η(eV)	ω(eV)
Thz1	3.427	2.915	2.014
Thz2	3.383	2.940	1.946
Thz3	3.370	2.957	1.920
Thz4	3.483	2.856	2.123
Thz5	3.621	2.721	2.410

In view of the results of Table 8, the compound Thz3 presents the smallest electronegativity value (χ=3.370 eV) of all our compounds. It is therefore the compound capable of giving up its electrons the fastest. The Thz5 compound has the smallest chemical hardness (η = 2.721 eV) which makes it the softest of all the compounds studied. With a low value of the electrophilic index (ω = 1.920 eV), the compound Thz3 is the one that receives the least electrons.

4. Conclusion

The theoretical study carried out on the five (05) compounds of the Thiazine family. using the methods of Quantum Chemistry and Molecular Modeling. made it possible to show that the compound Thz3 is the most stable and the one which yields with difficulty the electrons through the use of global reactivity descriptors. The Fukui indices and the dual descriptors made it possible to precisely determine attack sites. The latter showed that the sulfur atoms of the Thiazine ring are the electrophilic sites and those of nitrogen of the nucleus of Thiazine are the nucleophilic sites. For the rest of this work, we plan to study the stability of these compounds in solvents and then do an NBO study.

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