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Theoretical Study of Reactivity and Stability of a Thiazoline Derivative Series by the Density Functional Theory Method

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Abstract: This reactivity and stability work was performed on six (6) Thiazoline derivatives using density functional theory at the B3LYP/6-31+ G (d, p) level. The aim was to determine the electrophilic and nucleophilic sites and the chemical behaviour of thiazolines. To do this, we calculated the fukui reactivity parameters (f+; f-), as well as the conceptual DFT reactivity parameters. The analysis of local descriptors and the molecular electrostatic potential map identified the nitrogen (N) atoms of the Thiazoline ring as the preferred electrophilic attack site (nucleophilic site) for the compound series. Moreover, the Natural Population Analysis (NPA) also corroborated this same information, that is to say the sulfur atoms (S) are electrophilic sites and the nitrogen atoms the nucleophilic sites of the compounds studied. Also, the sulfur atones that bind the linker were designated as the nucleophilic attack site (electrophilic site). The study of the boundary molecular orbitals, including energy gap (ΔE), electronegativity (χ), chemical hardness (η), and electrophilicity index (ω) allowed the chemical reactivity of Thiazoline derivatives to be described from the molecular properties. Thus, the Th3 molecule is the most stable, least reactive and hardest. Moreover, the Th3 compound is the one which gives the least electrons on all the studied molecules.

Keywords: Local Reactivity, Global Reactivity, Thiazoline, DFT

1. Introduction

Thiazolines are a group of isomeric 5-membered heterocyclic compounds containing both sulfur and nitrogen in the ring. Unsubstituted thiazolines are rarely found by themselves, their derivatives are more common and some are bioactive [1].

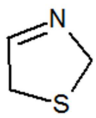
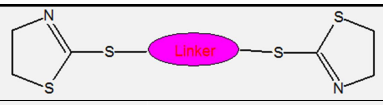


Figure 1. *Structure of Thiazoline.*

Five- and six-membered nitrogen-containing heterocyclic compounds such as oxazolines, thiazolines and thiazines are of great interest to chemists because they have interesting biological properties [2-5]. Nowadays, computational chemistry provides a lot of information about the electronic structures of molecules and contributes greatly to the development of traditional experimental chemistry [6, 7]. This technique is widely used to reduce the number of experiments, sometimes long, dangerous and costly in terms of time and money [8, 9]. The general objective of this work is to determine theoretically, the reactivity, to identify the nucleophilic/electrophilic attack sites by different methods of quantum chemistry.

Table 1. *Structures of the studied Thiazoline derivatives.*



Code	Linker
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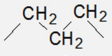
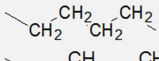
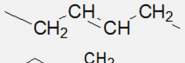
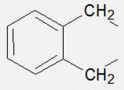
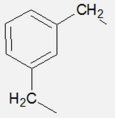
Th2	
Th3	
Th4	
Th5	
Th6	

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 [10-12] in the 6-31+G (d, p) basis using the Gaussian 09 software [13]. This Hybrid functional gives better energies and is in agreement with high level ab initio methods [14, 15]. The geometries are held constant for both cationic and anionic systems. The global reactivity indices were obtained from the conceptual DFT model [16, 17, 7].

2.2. Reactivity Descriptors

2.2.1. 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) (E_{LUMO}), the energy of the highest occupied molecular orbital (MO) (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 [18]. 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):

$$I = -E_{HOMO} \quad (1)$$

$$A = -E_{LUMO} \quad (2)$$

$$\chi = -\mu = -1/2\,(E_{LUMO} + E_{HOMO}) \quad (3)$$

$$\eta = (E_{LUMO} - E_{HOMO})/2 \quad (4)$$

$$\omega = \frac{\chi^2}{2\eta} \quad (5)$$

$$\sigma = 1/\eta \quad (6)$$

2.2.2. Local Descriptors 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 [19]. 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 [20] 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^-) [21] have been determined. The Fukui functions are calculated using equations (7) and (8):

$$f_k^+ = q_k(N+1) - q_k(N) \quad (7)$$

$$f_k^- = q_k(N) - q_k(N-1) \quad (8)$$

f_k^+ for nucleophilic attack.

f_k^- for electrophilic attack.

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

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

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

The values of the dual descriptors [22, 23] are obtained from equations (13 to 15).

$$\Delta f = f_k^+ - f_k^- \quad (9)$$

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 [24]. 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. Map of the Electrostatic Potential

The surface of the molecular electrostatic potential (MEP) is illustrated by the colors that vary from red to blue. Areas that have zero potential are represented by the color green. The potential increases in the order red < orange < yellow < green < cyan < blue [25, 26]. In the MEP surface, the negative areas (red and yellow) of the MEP are electrophilic attack sites and the positive areas (cyan and blue) are nucleophilic attack sites.

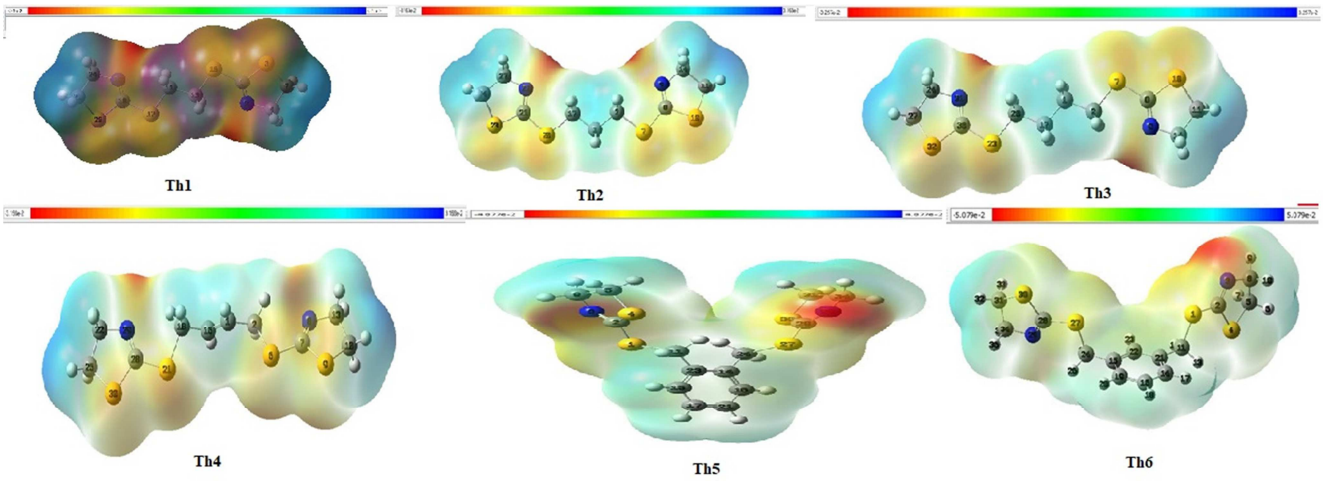
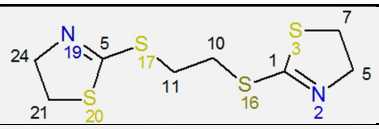


Figure 2. *Molecular Electrostatic Potential (MEP) surface of compounds Th1 to Th6.*

3.1.2. Determination of Electrophilic and Nucleophilic Sites

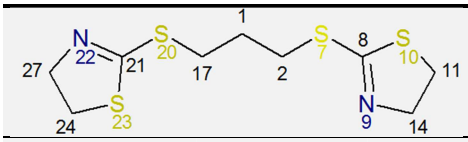
The study of determination of electrophilic and nucleophilic sites of the six (6) molecules derived from Thiazoline was conducted, by calculating the Fukui indices (f^+, f^-) and the dual descriptor ($\Delta f(r)$) (Tables 2 to 7).

Table 2. *Local reactivity descriptors of compound Th1 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d, p) level.*

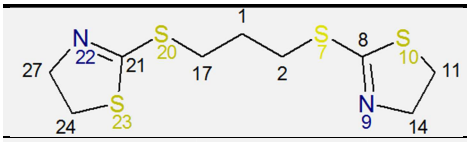


Atoms	Q (N)	Q (N+1)	Q (N-1)	f+	f-	Δf (r)
C1	6.089	6.032	6.096	-0.057	-0.007	-0.051
N2	7.510	7.267	7.073	-0.243	0.437	-0.680
S3	15.759	15.874	15.693	0.115	0.066	0.049
C4	6.306	6.147	6.163	-0.160	0.143	-0.303
C7	6.621	6.294	6.314	-0.327	0.307	-0.634
C10	6.615	6.298	6.314	-0.318	0.302	-0.620
C11	6.615	6.298	6.314	-0.318	0.302	-0.620
S16	15.687	15.843	15.734	0.156	-0.047	0.203
S17	15.687	15.843	15.734	0.156	-0.047	0.203
C18	6.089	6.032	6.096	-0.057	-0.007	-0.051
N19	7.510	7.267	7.073	-0.243	0.437	-0.680
S20	15.759	15.874	15.693	0.115	0.066	0.049
C21	6.621	6.294	6.314	-0.327	0.307	-0.634
C24	6.306	6.147	6.163	-0.160	0.143	-0.303

Table 3. *Local reactivity descriptors of compound Th2 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d, p) level.*

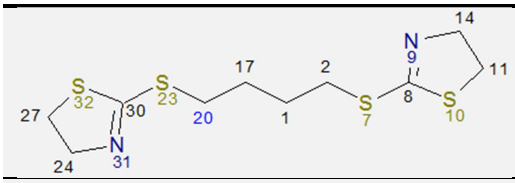


Atoms	Q (N)	Q (N+1)	Q (N-1)	f+	f-	Δf (r)
C1	6.504	6.246	6.255	-0.258	0.249	-0.506
C2	6.597	6.288	6.304	-0.309	0.293	-0.602
S7	15.691	15.847	15.737	0.156	-0.046	0.202
C8	6.089	6.037	6.095	-0.052	-0.006	-0.046
N9	7.511	7.263	7.077	-0.248	0.435	-0.683



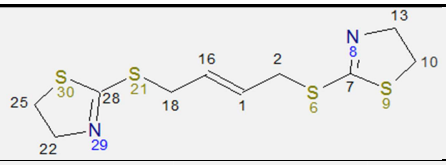
Atoms	Q (N)	Q (N+1)	Q (N-1)	f+	f-	Δf (r)
S10	15.760	15.877	15.693	0.117	0.067	0.050
C11	6.622	6.292	6.315	-0.330	0.307	-0.637
C14	6.306	6.146	6.163	-0.160	0.144	-0.303
C17	6.597	6.288	6.304	-0.309	0.293	-0.602
S20	15.691	15.847	15.737	0.156	-0.046	0.202
C21	6.089	6.037	6.095	-0.052	-0.006	-0.046
N22	7.511	7.263	7.077	-0.248	0.435	-0.683
S23	15.760	15.877	15.693	0.117	0.067	0.050
C24	6.621	6.292	6.315	-0.330	0.307	-0.637
C27	6.306	6.146	6.163	-0.160	0.144	-0.303

Table 4. *Local reactivity descriptors of compound Th3 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d, p) level.*



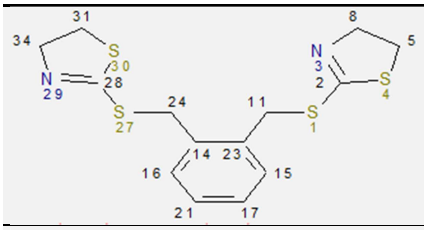
Atoms	Q (N)	Q (N+1)	Q (N-1)	f+	f-	Δf(r)
C1	6.486	6.238	6.245	-0.247	0.241	-0.488
C2	6.596	6.292	6.302	-0.304	0.294	-0.597
S7	15.694	15.851	15.738	0.158	-0.045	0.202
C8	6.089	6.037	6.095	-0.052	-0.006	-0.046
N9	7.512	7.264	7.075	-0.247	0.436	-0.684
S10	15.762	15.874	15.696	0.112	0.065	0.047
C11	6.622	6.291	6.315	-0.331	0.307	-0.637
C14	6.306	6.146	6.163	-0.160	0.143	-0.304
C17	6.486	6.238	6.245	-0.247	0.241	-0.488
C20	6.596	6.292	6.302	-0.304	0.294	-0.597
S23	15.694	15.851	15.738	0.158	-0.045	0.202
C24	6.306	6.146	6.163	-0.160	0.143	-0.304
C27	6.622	6.291	6.315	-0.331	0.307	-0.637
C30	6.089	6.037	6.095	-0.052	-0.006	-0.046
N31	7.512	7.264	7.075	-0.247	0.436	-0.684
S32	15.762	15.874	15.696	0.112	0.065	0.047

Table 5. *Local reactivity descriptors of compound Th4 calculated using natural population analysis (NPA) at the DFT/ B3LYP/6-31+G (d, p) level.*



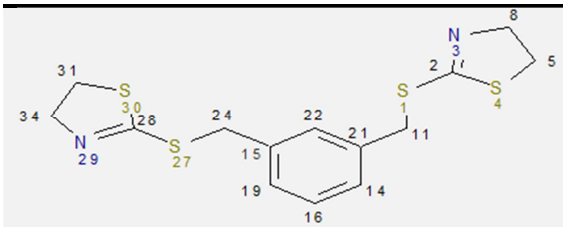
Atoms	Q (N)	Q (N+1)	Q (N-1)	f+	f-	Δf(r)
C1	6.228	6.093	6.105	-0.136	0.123	-0.259
C2	6.618	6.296	6.312	-0.322	0.306	-0.628
S6	15.691	15.842	15.761	0.151	-0.070	0.221
C7	6.090	6.037	6.092	-0.053	-0.003	-0.050
N8	7.514	7.263	7.084	-0.251	0.431	-0.682
S9	15.759	15.889	15.678	0.130	0.081	0.049
C10	6.621	6.296	6.315	-0.325	0.306	-0.632
C13	6.306	6.147	6.163	-0.159	0.144	-0.302
C16	6.225	6.089	6.113	-0.136	0.112	-0.248
C18	6.620	6.299	6.313	-0.322	0.307	-0.629
S21	15.693	15.843	15.736	0.150	-0.043	0.194
C22	6.306	6.148	6.163	-0.158	0.143	-0.301
C25	6.621	6.292	6.314	-0.329	0.307	-0.637
C28	6.088	6.037	6.095	-0.051	-0.007	-0.044
N29	7.515	7.262	7.074	-0.253	0.440	-0.693
S30	15.758	15.889	15.698	0.131	0.060	0.071

Table 6. *Local reactivity descriptors of compound Th5 calculated using natural population analysis (NPA) at DFT/ B3LYP/6-31+G (d, p) level.*



Atoms	Q (N)	Q (N+1)	Q (N-1)	f+	f-	Δf (r)
S1	15.680	15.848	15.675	0.168	0.005	0.163
C2	6.091	6.028	6.098	-0.062	-0.008	-0.055
N3	7.488	7.241	7.063	-0.247	0.426	-0.673
S4	15.780	15.894	15.771	0.115	0.008	0.106
C5	6.620	6.302	6.311	-0.318	0.309	-0.627
C8	6.308	6.151	6.165	-0.157	0.143	-0.300
C11	6.613	6.297	6.306	-0.315	0.307	-0.622
C14	6.050	6.028	6.033	-0.023	0.017	-0.039
C15	6.218	6.072	6.105	-0.147	0.114	-0.261
C16	6.218	6.072	6.105	-0.147	0.114	-0.261
C17	6.234	6.118	6.107	-0.116	0.127	-0.243
C21	6.234	6.118	6.107	-0.116	0.127	-0.243
C23	6.050	6.028	6.033	-0.023	0.017	-0.039
C24	6.613	6.297	6.306	-0.315	0.307	-0.622
S27	6.680	6.848	6.675	0.168	0.005	0.163
C28	6.091	6.028	6.098	-0.062	-0.008	-0.055
N29	6.488	6.241	6.063	-0.247	0.426	-0.673
S30	5.780	5.894	5.771	0.115	0.008	0.106
C31	6.620	6.302	6.311	-0.318	0.309	-0.627
C34	6.308	6.151	6.165	-0.157	0.143	-0.300

Table 7. *Local reactivity descriptors of compound Th6 calculated using natural population analysis (NPA) at DFT/ B3LYP/6-31+G (d, p) level.*



Atoms	Q (N)	Q (N+1)	Q (N-1)	f+	f-	Δf(r)
S1	15.670	15.835	15.677	0.165	-0.007	0.172
C2	6.091	6.035	6.098	-0.055	-0.008	-0.048
N3	7.488	7.249	7.054	-0.239	0.434	-0.673
S 4	15.789	15.895	15.757	0.107	0.031	0.075
C5	6.620	6.302	6.312	-0.318	0.308	-0.626
C8	6.308	6.150	6.165	-0.158	0.143	-0.300
C11	6.607	6.292	6.306	-0.315	0.301	-0.616
C14	6.223	6.076	6.107	-0.147	0.115	-0.263
C15	6.063	6.013	6.033	-0.050	0.030	-0.081
C16	6.233	6.137	6.096	-0.096	0.137	-0.233
C19	6.221	6.077	6.104	-0.145	0.117	-0.262
C21	6.063	6.014	6.036	-0.049	0.027	-0.076
C22	6.205	6.115	6.091	-0.091	0.114	-0.205
C24	6.594	6.284	6.300	-0.310	0.294	-0.604
S27	15.686	15.834	15.749	0.149	-0.064	0.212
C28	6.092	6.041	6.091	-0.051	0.001	-0.052
N29	7.514	7.263	7.095	-0.251	0.419	-0.669
S30	15.760	15.890	15.717	0.130	0.043	0.088
C31	6.622	6.298	6.314	-0.324	0.308	-0.631
C34	6.306	6.150	6.162	-0.157	0.144	-0.301

The analysis of the different tables (Tables 2 to 7) shows that the sulfur (S) atoms that link the linker have the largest values of the dual descriptor. This result implies that these sulfur atoms (S) are electrophilic sites of the studied Thiazoline derivatives. Also, the lowest values of the dual descriptor are attributed to the nitrogen (N) atoms of the Thiazoline ring. These low values reflect that these nitrogen atoms are the nucleophilic sites of the studied Thiazoline derivatives. These different sites are illustrated in Figure 3.

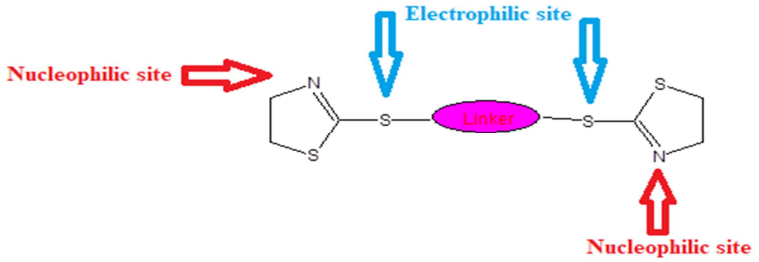


Figure 3. *Representation of the electrophilic and nucleophilic sites of Thiazoline derivatives.*

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 8.

Table 8. *Energy descriptors of the studied compounds.*

MOLECULES	E (HOMO) (eV)	E (LUMO) (eV)	ΔE (eV)	I (eV)	A (eV)
Th1	-6.518	-0.643	5.874	6.518	0.643
Th2	-6.493	-0.550	5.943	6.493	0.550
Th3	-6.464	-0.431	6.032	6.464	0.431
Th4	-6.486	-0.870	5.616	6.486	0.870
Th5	-6.347	-0.570	5.777	6.347	0.570
Th6	-6.338	-1.065	5.273	6.338	1.065

The values in Table 8 indicate that the Th3 molecule has the largest energy gap value (ΔE=6.032 eV), making this compound the least reactive and most stable of the Thiazoline series studied. In contrast to the compound Th6 which has the smallest energy gap (ΔE=5.273 eV), thus more reactive and less stable. Thus, the following sequence can be established in order of decreasing stability:

ΔE: Th3 > Th2>Th1> Th5> Th4>Th6

The boundary molecular orbitals (HOMO and LUMO) of Thiazoline derivatives obtained using the B3LYP/6-31+G (d, p) method are shown in Figure 4.

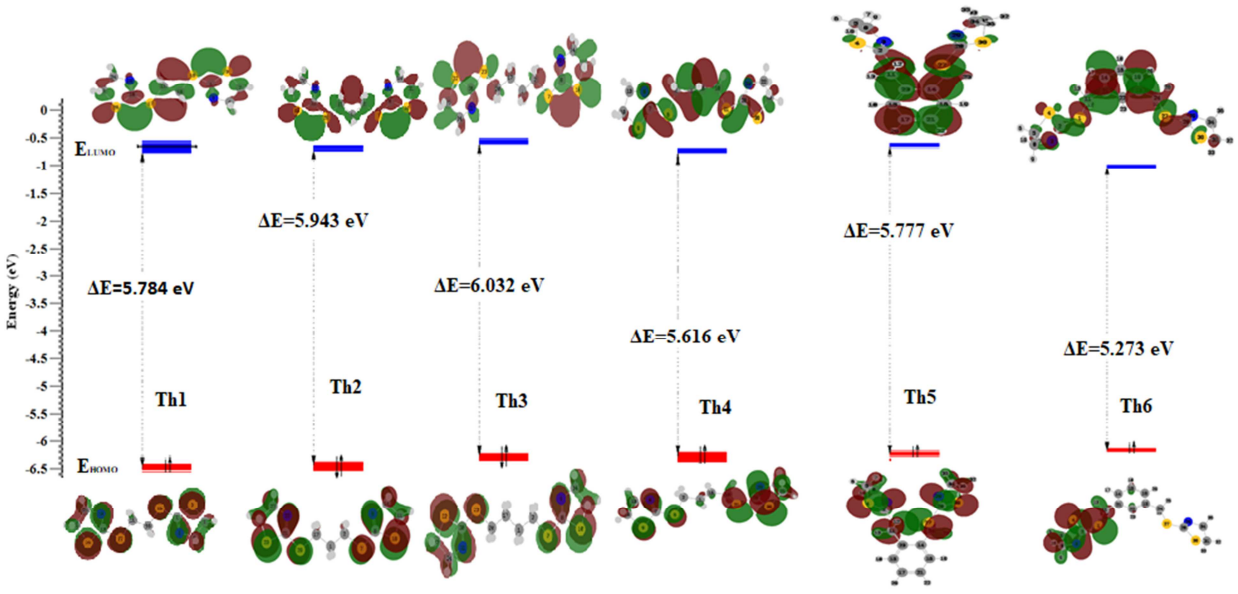


Figure 4. *Highest occupied and lowest vacant molecular orbitals of Th1 to Th6 compounds.*

The overall reactivity indices of the Thiazoline derivatives studied are shown in Table 9.

Table 9. *Global descriptors of chemical reactivity of Th1 to Th6 compounds.*

MOLECULES	χ (eV)	η (eV)	ω (eV)
Th1	3.580	2.937	2.182
Th2	3.521	2.972	2.086
Th3	3.448	3.016	1.970
Th4	3.678	2.808	2.409
Th5	3.458	2.888	2.070
Th6	3.701	2.636	2.598

The analysis of the values of the table shows us that with regard to the electronegativity χ, the compound Th3 has the lowest value (χ=3.448 eV) compared to the other molecules. This molecule is thus the one able to provide quickly its electrons. As for the chemical hardness (η), the compound Th6 has the lowest value (η=2.636 eV), which indicates that it is the softest of the compounds, therefore confirms that it is the most reactive. At the level of the electrophilicity index (ω), the compound Th3 presents lower value (ω=1.970 eV). This value confirms that this compound is less able to receive electrons.

4. Conclusion

Quantum chemistry methods were used on six (6) Thiazoline derivatives to study their chemical stability and reactivity. This work was performed using the DFT method at the B3LYP/6-31+G (d, p) level of theory. The analysis of local descriptors allowed us to determine the electrophilic and nucleophilic sites of the studied molecules. The Fukui indices and the dual descriptor were calculated from the natural charges. These showed that for Thiazoline derivatives, the linker-bound sulfur atoms are the electrophilic sites and the nitrogen atoms of the Thiazoline ring are the nucleophilic sites. The analysis of the overall descriptors revealed that the Th3 compound is the most stable, least reactive and hardest. On the other hand, the Th3 compound is the least electron donating among the studied compounds. As perspectives, we plan to carry out a dimerization study of these compounds.

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