Review Article

THEORETICAL STUDY OF THE CHEMICAL REACTIVITY OF A SERIES OF 2,3-DIHYDRO-1H-PERIMIDINE.

Abstract

This reactivity study was performed on seven molecules of a 2,3-dihydro-1H-perimidine series using density functional theory, at the B3LYP / 6-311 G (d, p) level. Calculation of the dipole moment showed that compound 5 is more soluble in aqueous medium. The study of frontier molecular orbitals, in particular the energy gap (ΔE), electronegativity (χ), chemical hardness (η) and the electrophilic index (ω) has provided a better overview molecular properties. Thus, the compound 5 with the highest energy gap between the boundary orbitals is the most stable and the least reactive. Analysis of local descriptors and the electrostatic potential map identified nitrogen atoms N_{26} and N_{28} as the preferred sites of electrophilic attack and the carbon atom C26 as the preferred site of nucleophilic attack.

Comment [L1]: 4

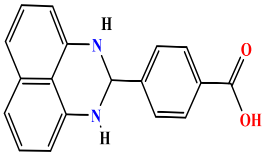
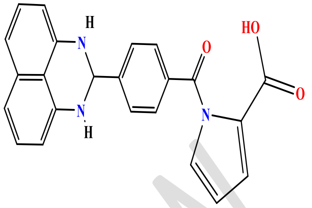
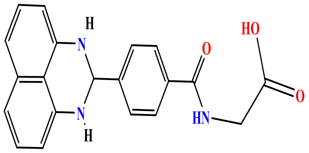
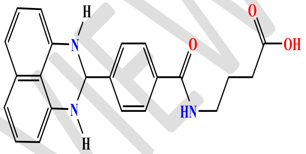
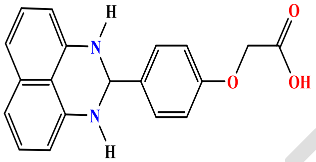
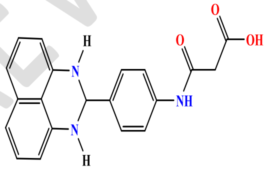
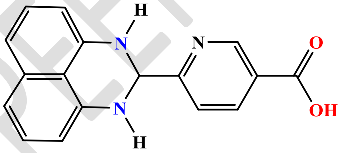
keyword: Reactivity, 2,3-dihydro-1*H*-perimidine, Fukui function, Natural charge, DFT

Introduction

The heterocycles are chemical compounds whose carbon chain consists of rings in which one or more carbon atoms can be replaced by a heteroatom such as nitrogen, oxygen, phosphorus, sulfur, etc. These chemical compounds are of great scientific interest because of their potential for application in many fields. The most well-known are heterocycles containing nitrogen and oxygen atoms [1]. Among others, we can mention 2,3- dihyro -1*H* -Perimidines are defined as the product resulting from the condensation of 1,8-diaminonaphthalene (1,8 - DAN) with carbonyl derivatives (Aldehyde). The 1*H* - perimidines which are heterocyclic compounds constitute a class of organic compounds which has a great structural variety. This allows their use in various scientific fields. They are characterized by either a bond deficit or an excess Π bond due to the electron density movements of the nitrogen atoms present in the naphthalene ring [2]. These compounds have a very important interest because of their polyvalent [3], optoelectronic, chemotherapeutic, thermochromic, and photochromic properties. In this work, a series of seven (7) molecules of 2,3-dihydro-1*H*-perimidine were used (Table 1). The aim of this work is to theoretically determine, on the one hand, the reactivity of 2,3-dihydro-1*H*-perimidine and on the other hand to identify the sites of nucleophilic / electrophilic attacks by different methods of quantum chemistry.

Comment [L2]: dihydro

Table 1: Molecular structure of 2,3-dihydro-1*H*-perimidine studded

Compounds	Structures	Compounds	Structures
1		2	
3		4	
5		6	
7			

2. Material and Methods

2.1. Natural Population Analysis

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 [4]. In this work, the atomic charge values were obtained by the Natural population analysis. The geometry of the molecules was optimized by the DFT calculation method with the B3LYP functional [5] in the basis 6-311G (d, p) using the Gaussian 09 [6]. This Hybrid functional gives better energies and is in line with high-level ab initio methods [7]. The geometries are conserved for cationic and anionic systems at computational level B3LYP/6-311G (d, p) to which a calculation of energy has been made.

2.2. Frontier Molecular Orbitals Theory

The frontier molecular orbital play a fundamental role in the qualitative interpretation of chemical reactivity [8]. The highest occupied molecular orbital (HOMO), which is considered to be the outer electron-containing orbital, tends to give these electrons as an electron donor. On the other hand, the lowest vacant molecular orbital (LUMO) is perceived as the lowest orbital containing free places to accept electrons. While the energy of the HOMO is directly related to the ionization potential, that of the LUMO is directly related to the electronic affinity. The difference in energy between the HOMO and the LUMO, called the energy gap, is an important stability factor for structures. The HOMO-LUMO energy gap helps characterize the chemical reactivity and kinetic stability of the molecule [8]. A molecule with a high energy gap (ΔE) is less polarizable and is generally associated with low chemical reactivity and high kinetic stability [9]

2.3. Reactivity Descriptors
2.3.1. Global Descriptors

Some theoretical descriptors related to conceptual DFT have been determined to predict chemical reactivity. These are ionization potential (I), electron affinity (A), the electronegativity (χ), global Softness (s), global hardness (η) and global electrophilicity (ω) [10]. These descriptors are all determined from the optimized molecules. It should be noted that the descriptors related to the molecular frontier orbitals have been calculated as part of the Koopmans approximation [11]. The LUMO energy which 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. Electronegativity (χ) is the parameter that reflects the ability of a molecule not to let its electrons escape. Global softness (s) expresses the resistance of a system to the change in its number of electrons. The overall electrophilicity index characterizes the electrophilic power of the molecule. These different parameters are calculated from equations (1):

$$
\begin{gathered}
I = -E_{HOMO} \\
A = -E_{LUMO} \\
\chi = -\mu = -1/2\,(E_{LUMO} + E_{HOMO}) \\
\eta = (E_{LUMO} - E_{HOMO})/2 \qquad (1) \\
\omega = \frac{\chi^2}{2\eta} \\
\sigma = 1/\eta
\end{gathered}
$$

The chemical potential (μ) is defined as the escaping tendency of electron from equilibrium while (χ) describes the ability of a molecule to attract electrons towards itself in a covalent bond. With regard to the global hardness, it measures the resistance towards the deformation or polarization of the electron cloud of the atoms, ions or molecules under small perturbation of chemical reaction. Parr and et al. introduced the concept of Electrophilicity as a global reactivity index similar to the chemical hardness and chemical potential.

2.3.2. Local and Dual Descriptors

Fukui indices of a molecule inform about the local reactivity in a molecule. The atom with the largest Fukui index is more reactive than the other constituent atoms of the molecule [12]. These indices represent the qualitative description of the reactivity of the atoms in the molecule. Fukui's function successfully predicts the relative reactivity for most chemical systems. The determination of the Fukui indices for the selectivity of electrophilic and nucleophilic atoms in the perimidine compounds has been made. Ayers and Parr [13] explained that molecules tend to react where Fukui's function is greatest when attacked by soft reagents and in places where Fukui's function is smaller when attacked by hard reagents. Using the natural atomic charge of the ground state optimized compounds, the Fukui function (f_k^+ f_k^-), the local softness (s_k^+, s_k^-) and the local electrophilia indices (ω_k^+, ω_k^-) [14] have been determined. The functions of Fukui are calculated using equation (2):

$$f_k^+ = q_k(N+1) - q_k(N)$$
$$f_k^- = q_k(N) - q_k(N-1) \quad (2)$$

f_k^+: for nucleophilic attack
f_k^-: for electrophilic attack
$q_k(N)$: Electron population of the atom k in the neutral molecule.
$q_k(N+1)$: Electron population of the atom k in the anionic molecule.
$q_k(N-1)$: Electron population of the atom k in the cationic molecule.

Local softness and electrophilicity indices are calculated using (3)

$$\begin{aligned} s_k^+ &= sf_k^+ \\ s_k^- &= sf_k^- \\ \omega_k^+ &= \omega f_k^+ \\ \omega_k^- &= \omega f_k^- \end{aligned} \quad (3)$$

The values of the dual descriptors [15] are obtained from the equations (4)

$$\Delta f = f_k^+ - f_k^- \quad (4)$$

3. Results and Discussion

3.1. Dipoles moment of compounds μ (D).

The dipole moment is an essential parameter for the prediction of the solubility of compounds in aqueous medium. The values of the dipole moment are reported in Table 2.

Table 2: Dipoles moment of compounds

compounds	1	2	3	4	5	6	7
μ (D)	0.793	4.077	4.618	4.154	4.828	4.180	4.758

The dipole moment values of the compounds range from 0.793 Debye to 4.828 Debye. The decreasing order of the dipole moment of the compounds is as follows:

μ (Compound 5)> μ (Compound 7)> μ (Compound 3)> μ (Compound 6)> μ (Compound 4)> μ (Compound 2)> μ (Compound 1).

The order shows us that compound 5 has the greatest dipole moment value. Compound 5 is therefore more soluble in aqueous medium.

3.2. Analysis of frontier molecular orbital

Below shows the HOMO and LUMO boundary molecular orbital patterns of the 2,3-dihydro-1*H*-perimidine obtained using the B3LYP/6-311G (d, p) method.

The analysis of the frontier orbital indicates that the HOMO of the compounds is around of the cycle of naphthalene in which contains the system non planar at six-member and the tow azote atom. The LUMO covers most of the carbon atoms of the cycle phenyl.

Table 3: Energy parameters of the compounds studied

compounds	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔEgap (eV)	EI (eV)	A (eV)
1	-4.905	-1.597	3.308	4.905	1.597
2	-4.884	-1.958	2.926	4.884	1.958
3	-4.838	-1.276	3.562	4.838	1.276
4	-4.790	1.179	5.969	4.790	-1.179
5	-4.759	-0.547	4.211	4.759	0.547
6	-4.812	-1.739	3.073	4.812	1.739
7	-4.731	-0.670	4.060	4.731	0.670

The energy parameters obtained from the energies of the frontier orbital are grouped in Table 3. These results show that Compound 2 has the smallest energy gap (ΔEgap = 2.926 eV), so it is the most polarizable, has the highest chemical reactivity and the lowest kinetic stability with respect to all studied molecules. In contrast, compound 4 has the largest value of the energy gap of 5.969 eV. The compound 2 is therefore most polarizable, with high chemical reactivity ant low kinetic on the seven (07) compounds studied.

3.3. Reactivity descriptors

3.3.1. Global reactivity descriptors

In This study of the global reactivity of molecules is based on the calculation of global indices deduced from electronic properties. The overall indices of the reactivity of the 2,3-dihydro-1*H*-perimidine studied were calculated from Equations (1) and recorded in Table 4.

The value of the overall hardness of compound 2 (η = 1.463 eV) is the lowest of all molecules. Thus, it appears that the compound 2 is more reactive than all the compounds studied. Also, we note that compound 2 has a significantly higher electronegativity value (χ = 3.421 eV) than other compounds; it is the best acceptor of electrons. In addition, the value of the electrophilic index of compound 2 (ω = 4.000 eV) indicates that it is the most electrophilic.

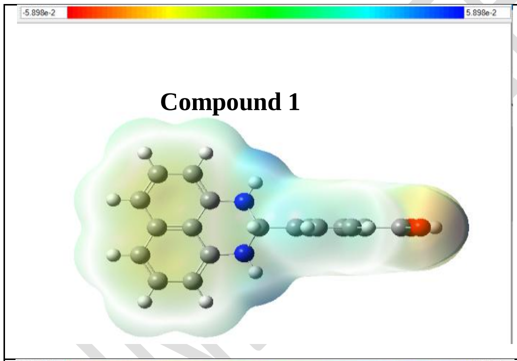
Table 4: Global descripteurs of chemical reactivity of 2,3-dihydro-1H-perimidine 1-

compounds	μ(eV)	η(eV)	ω(eV)	χ(eV)	s(eV^{-1})
1	-3.251	1.654	3.195	3.251	0.605
2	-3.421	1.463	4.000	3.421	0.683
3	-3.057	1.781	2.623	3.057	0.561
4	-1.806	2.985	0.546	1.806	0.335
5	-2.653	2.106	1.671	2.653	0.475
6	-3.276	1.537	3.491	3.276	0.651
7	-2.701	2.030	1.796	2.701	0.493

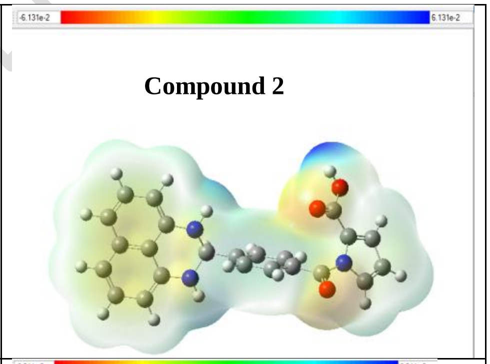
3.3.2. Local reactivity descriptors

3.3.2.1 Molecular Electrostic potentials and fukui functions

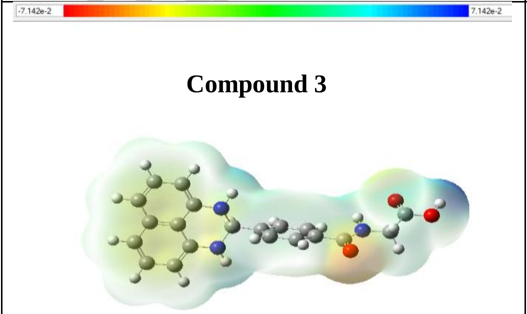
The different areas of the electrostatic surface potential are represented by colors ranging from red to blue. The potential increases in order red <orange <yellow <green <blue, where red indicates the most negative potentials and blue the most positive potentials [16] passing successively through orange, yellow and green. The surfaces of the electrostatic potentials of the studied molecules were represented after optimization at the level DFT/B3LYP / 6-311 G (d, p). They are presented in Figure 1 obtained from Gaussian 09 [6].



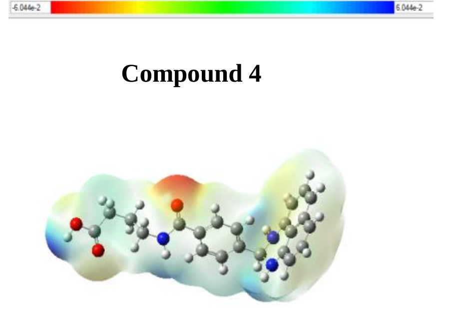
Compound 1



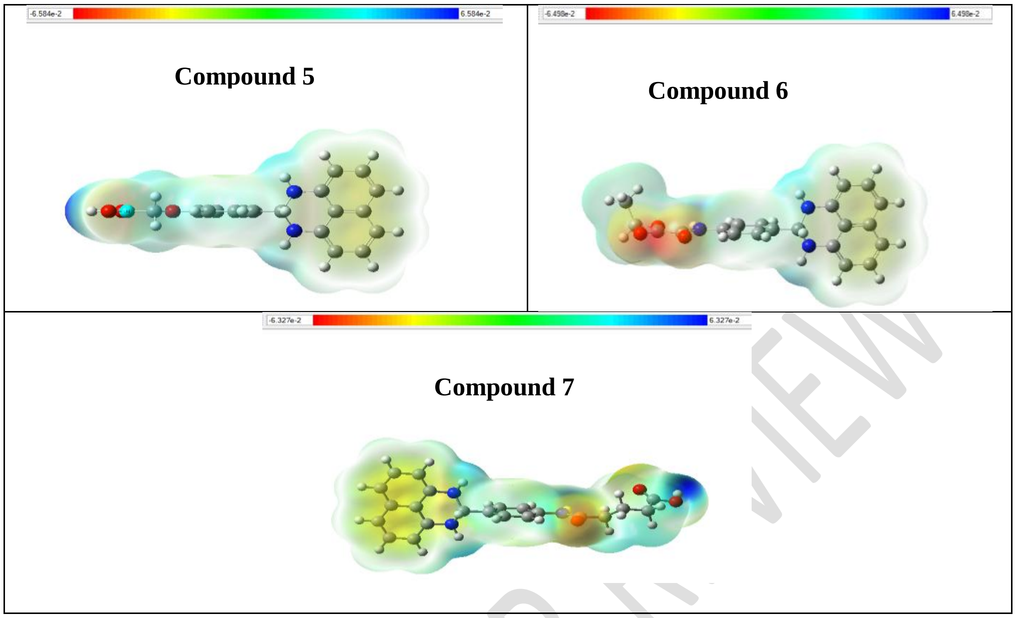
Compound 2



Compound 3



Compound 4



Compound 5

Compound 6

Compound 7

Figure 1: Surface of molecular Electrostic potentials of 2,3-dihydro-1*H*-perimidine

Local indices of reactivity were also determined for each molecule according to equations (2), (3) and (4). All the atoms of compounds are concerned in this study except the hydrogen atoms. These different local indices and descriptors of reactivity are grouped in Tables 5 to 11.

The values of the local descriptors of compound 1 calculated at B3LYP/6-311G (d, p) show that the azote atoms N_{26} and N_{28} are the preferred sites of electrophilic attack. According to this same level of calculation, a nucleophilic attack will preferably take place on the C_{32} atom having a value in the Table 5.

Table 5: Compound 1 reactivity descriptors calculated using Natural Population Analysis (NPA)

Sites	Locals descriptors							
	f+	f-	ω+	ω-	s+	s-	η+	η-
C32	0.523	-0.419	0.966	-0.773	0.252	-0.201	0.602	-0.482
C10	0.128	-0.041	0.237	-0.076	0.062	-0.020	0.148	-0.048
C31	0.128	-0.041	0.237	-0.076	0.062	-0.020	0.148	-0.048
C30	0.079	-0.073	0.145	-0.135	0.038	-0.035	0.090	-0.084
C16	0.133	0.006	0.245	0.010	0.064	0.003	0.153	0.006
C3	-0.027	-0.027	-0.049	-0.049	-0.013	-0.013	-0.031	-0.031
C5	-0.131	0.278	-0.241	0.512	-0.063	0.134	-0.150	0.320
O33	-0.200	0.310	-0.368	0.572	-0.096	0.149	-0.230	0.357
O34	-0.324	0.355	-0.597	0.655	-0.156	0.171	-0.372	0.408
N28	-0.312	0.419	-0.576	0.774	-0.150	0.202	-0.359	0.482

N26	-0.312	0.419	-0.576	0.774	-0.150	0.202	-0.359	0.482

The results in Table 6 predict that the N_{28} and N_{30} azote atoms are most favored for electrophilic attacks. As regards the nucleophilic attack, it occurs preferentially on carbon C_{26}.

Table 6: Compound 2 reactivity descriptors calculated using Natural Population Analysis (NPA)

Sites	Locals descriptors							
	f+	f-	ω+	ω-	s+	s-	η+	η-
C26	0.538	-0.367	0.993	-0.677	0.259	-0.176	0.619	-0.422
C42	0.425	-0.025	-0.450	0.476	-0.900	0.926	0.489	-0.029
C10	0.103	-0.043	0.190	-0.079	0.049	-0.021	0.118	-0.049
C33	0.103	-0.043	0.190	-0.079	0.049	-0.021	0.118	-0.049
C32	0.071	-0.073	0.132	-0.134	0.034	-0.035	0.082	-0.084
N34	-0.224	0.198	-0.413	0.366	-0.108	0.095	-0.258	0.228
O33	-0.277	0.296	-0.511	0.547	-0.133	0.142	-0.318	0.341
O34	-0.340	0.356	-0.627	0.657	-0.163	0.171	-0.391	0.410
N28	-0.319	0.418	-0.589	0.772	-0.153	0.201	-0.367	0.481
N30	-0.320	0.420	-0.590	0.776	-0.154	0.202	-0.368	0.484

In the Table 7, the azote atoms N_{28} and N_{30} are most favored for electrophilic attack. As regards the nucleophilic attack, are occurs preferentially on C_{26} and C_{39} carbon.

Table 7: Compound 3 reactivity descriptors calculated using Natural Population Analysis (NPA)

Sites	Locals descriptors							
	f+	f-	ω+	ω-	s+	s-	η+	η-
C26	0.417	-0.345	0.770	-0.636	0.201	-0.166	0.480	-0.397
C39	0.428	-0.004	-0.432	0.435	-0.863	0.867	0.492	-0.004
C10	0.138	-0.043	0.255	-0.080	0.067	-0.021	0.159	-0.050
C33	0.138	-0.043	0.256	-0.080	0.067	-0.021	0.159	-0.050
C32	0.083	-0.073	0.153	-0.136	0.040	-0.035	0.095	-0.085
O40	-0.299	0.303	-0.552	0.559	-0.144	0.146	-0.344	0.348
N34	-0.297	0.328	-0.549	0.605	-0.143	0.158	-0.342	0.377
O41	-0.341	0.351	-0.630	0.647	-0.164	0.169	-0.393	0.404
N30	-0.310	0.419	-0.572	0.774	-0.149	0.202	-0.357	0.483
N28	-0.310	0.420	-0.573	0.775	-0.1493	0.202	-0.357	0.483

Table 8 predicts that the N_{28} and N_{30} azote atoms are most favored against electrophilic attacks. As regards the nucleophilic attack, are occurs preferentially on C_{26} and C_{45} carbons.

Table 8: Compound 4 reactivity descriptors calculated using Natural Population Analysis (NPA)

Sites	Locals descriptors							
	f+	f-	ω+	ω-	s+	s-	η+	η-
C26	0.401	-0.349	0.740	-0.644	0.193	-0.168	0.462	-0.402
C45	0.437	-0.010	-0.447	0.46	-0.894	0.904	0.503	-0.012
C10	0.140	-0.052	0.258	-0.096	0.067	-0.025	0.161	-0.060
C33	0.139	-0.050	0.257	-0.093	0.067	-0.024	0.160	-0.058
C32	0.076	-0.077	0.141	-0.143	0.037	-0.037	0.088	-0.089
O46	-0.301	0.303	-0.556	0.559	-0.145	0.146	-0.347	0.349
N34	-0.297	0.333	-0.549	0.614	-0.143	0.160	-0.342	0.383
O47	-0.345	0.354	-0.636	0.654	-0.166	0.170	-0.397	0.408
N30	-0.307	0.414	-0.567	0.764	-0.148	0.199	-0.353	0.476
N28	-0.308	0.416	-0.568	0.768	-0.148	0.200	-0.354	0.479

The results in Table 9 predict that the N_{26} and N_{28} azote atoms are most favored for electrophilic attacks. As regards the nucleophilic attack, it occurs preferentially on carbon C_{36}.

Table 9: Compound 5 reactivity descriptors calculated using Natural Population Analysis (NPA)

Sites	Locals descriptors							
	f+	f-	ω+	ω-	s+	s-	η+	η-
C36	0.496	-0.078	-0.574	0.652	-1.148	1.226	0.571	-0.090
C23	0.165	-0.155	0.3045	-0.286	0.079	-0.075	0.190	-0.179
C31	0.188	-0.046	0.347	-0.085	0.090	-0.022	0.216	-0.053
C10	0.188	-0.046	0.347	-0.085	0.090	-0.022	0.216	-0.053
C30	0.089	-0.074	0.164	-0.137	0.043	-0.036	0.102	-0.086
O32	-0.244	0.258	-0.450	0.477	-0.117	0.124	-0.281	0.298
O37	-0.238	0.286	-0.440	0.528	-0.115	0.138	-0.274	0.329
O38	-0.342	0.359	-0.632	0.663	-0.165	0.173	-0.394	0.413
N28	-0.310	0.419	-0.573	0.774	-0.149	0.202	-0.357	0.483
N26	-0.310	0.419	-0.573	0.774	-0.149	0.202	-0.357	0.483

The values of the local descriptors calculated show that the azote atoms N_{26} and N_{28} are the preferred sites of electrophilic attack. According to this same level of calculation, a nucleophilic attack will preferably take place on the C_{32} atom having a value in the Table 10.

Table 10: Compound 6 reactivity descriptors calculated using Natural Population Analysis (NPA)

Sites	Locals descriptors							
	f+	f-	ω+	ω-	s+	s-	η+	η-
C32	0.494	-0.120	-0.615	0.735	-1.230	1.350	0.569	-0.139
C36	0.433	-0.137	-0.570	0.706	-1.140	1.276	0.499	-0.157
C23	0.120	-0.070	0.222	-0.129	0.058	-0.033	0.138	-0.080
C31	0.126	-0.045	0.233	-0.082	0.061	-0.021	0.145	-0.051
C10	0.126	-0.045	0.233	-0.082	0.061	-0.021	0.145	-0.051
O33	-0.163	0.279	-0.300	0.516	-0.078	0.134	-0.187	0.322
O38	-0.262	0.288	-0.484	0.532	-0.126	0.139	-0.302	0.331
N34	-0.317	0.305	-0.585	0.564	-0.152	0.147	-0.365	0.352
N28	-0.315	0.420	-0.582	0.776	-0.152	0.202	-0.363	0.484
N26	-0.315	0.420	-0.582	0.775	-0.152	0.202	-0.363	0.483

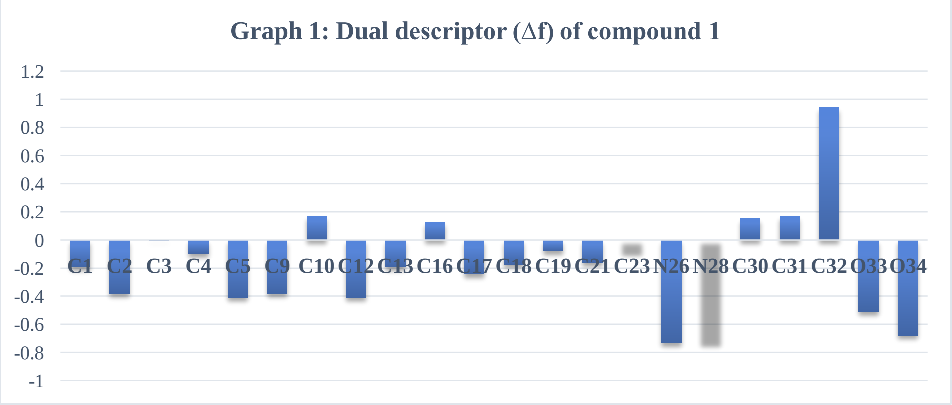
In the Table 11, the azote atoms N_{26} and N_{28} are most favored for electrophilic attack. As regards the nucleophilic attack, it occurs preferentially on C_{45} carbon.

Table 11: Compound 7 reactivity descriptors calculated using Natural Population Analysis (NPA)

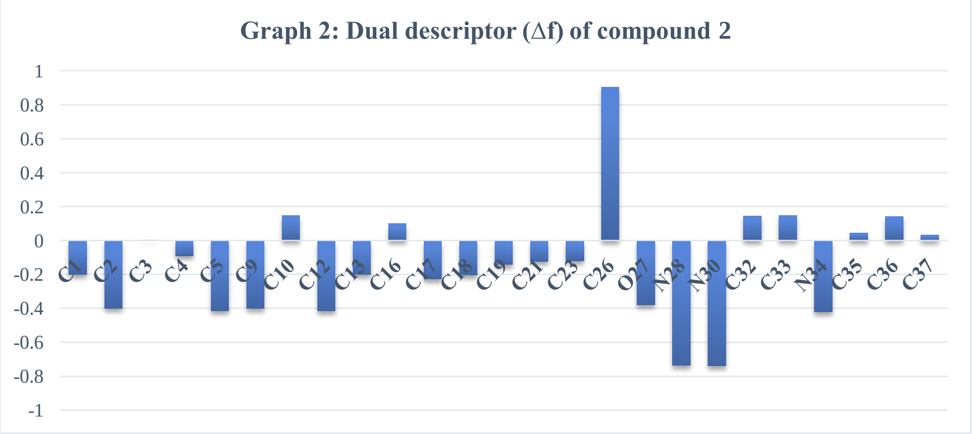
Sites	Locals descriptors							
	f+	f-	ω+	ω-	s+	s-	η+	η-
C45	0.520	-0.094	-0.614	0.708	-1.229	1.323	0.599	-0.108
C34	0.429	-0.071	-0.500	0.571	-1.000	1.071	0.493	-0.082
C23	0.146	-0.073	0.270	-0.134	0.070	-0.035	0.169	-0.084
C10	0.160	-0.047	0.295	-0.086	0.077	-0.022	0.184	-0.054
C31	0.160	-0.047	0.295	-0.086	0.077	-0.022	0.184	-0.054
O46	-0.299	0.301	-0.553	0.556	-0.144	0.145	-0.345	0.347
N32	-0.324	0.311	-0.599	0.574	-0.156	0.149	-0.373	0.358
O47	-0.325	0.354	-0.600	0.654	-0.156	0.170	-0.374	0.408
N28	-0.308	0.420	-0.568	0.775	-0.148	0.202	-0.354	0.483
N26	-0.308	0.420	-0.568	0.776	-0.148	0.202	-0.354	0.484

3.3.2.2. Dual reactivity descriptors.

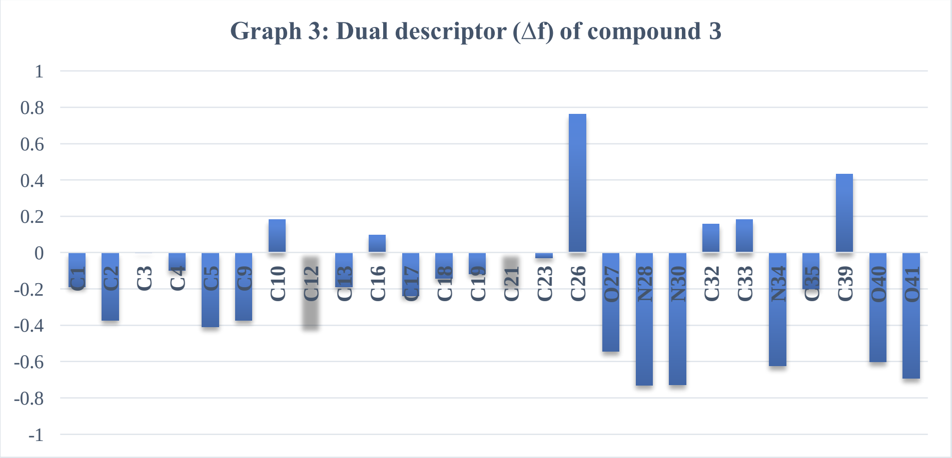
The numerical values of the dual reactivity descriptor were also determined for each molecule according to (2). All the constituent atoms of the different compounds are concerned in this study with the exception of the hydrogen atoms. These different local indices and descriptors of reactivity are grouped together in graphs 1 to 6 (Fig. 3). The numerical values of the double descriptor of the compounds were calculated at the level B3LYP / 6-311 G (d, p), show that the nitrogen atoms N_{26} and N_{28} for some compounds and N_{28} and N_{30} for others are generally the preferred sites of electrophilic attack.



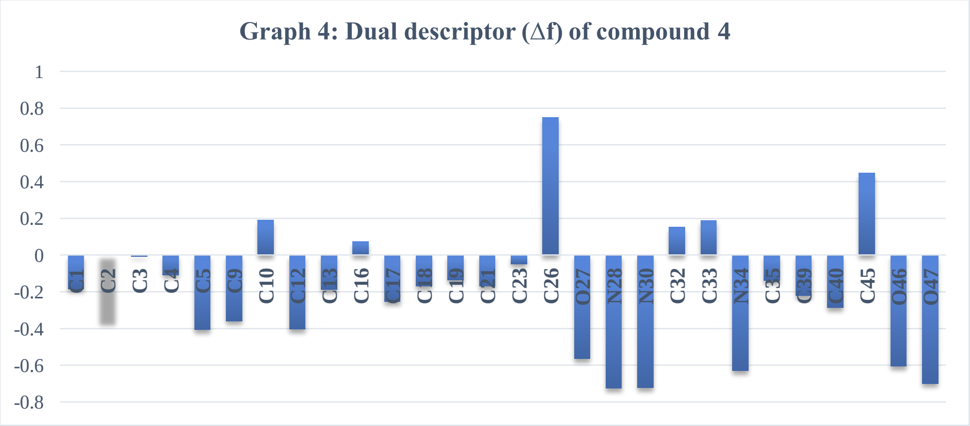
Graph 1: Dual descriptor (∆f) of compound 1



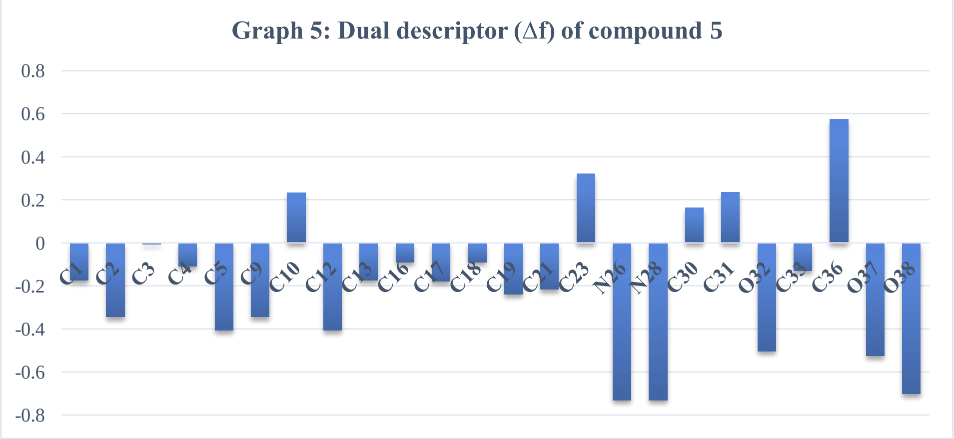
Graph 2: Dual descriptor (∆f) of compound 2



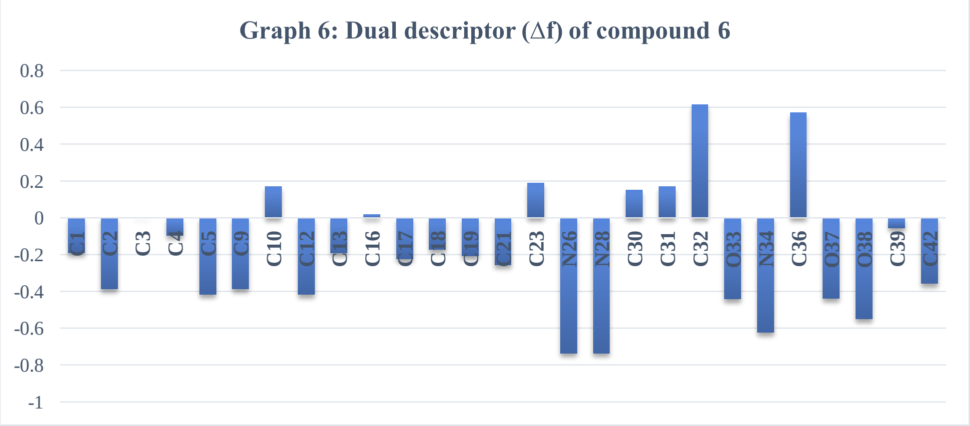
Graph 3: Dual descriptor (∆f) of compound 3



Graph 4: Dual descriptor (Δf) of compound 4



Graph 5: Dual descriptor (Δf) of compound 5



Graph 6: Dual descriptor (Δf) of compound 6

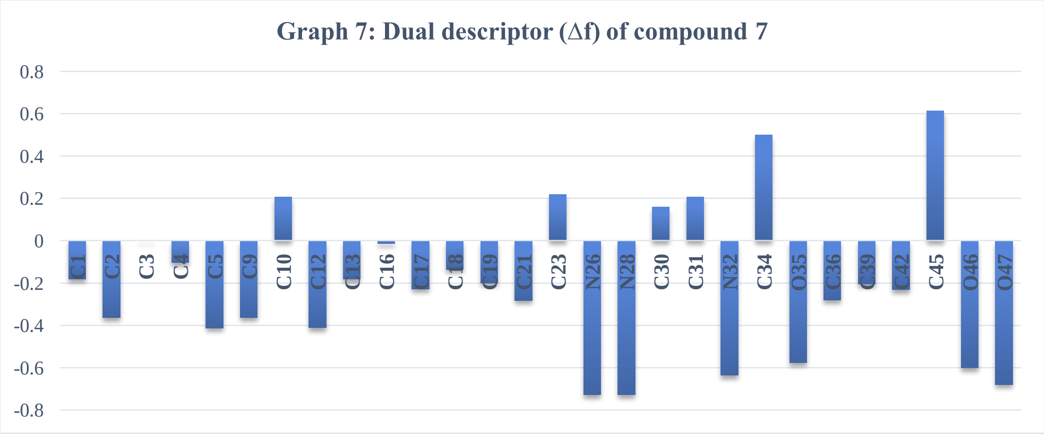


Figure 2: Values of the dual descriptor for the heavy atoms of compounds 1-7

Conclusion

In this work, the methods of Quantum Chemistry and Molecular Modeling were used on seven (7) molecules of the 2,3-dihydro-1H-perimidine family with a view to studying their reactivity. The dipole moment, global and local descriptors were used to study the reactivity of different nucleophilic, electrophilic and radical sites. The dipole moment showed that compound 5 is more soluble in aqueous medium. As for the global descriptors; they revealed that compound 4 is more stable and less reactive. Analysis of local descriptors confirmed the likely sites of electrophilic and nucleophilic attack. In order to accurately determine the sites of attack, the Fukui indices and dual descriptors were calculated from the Natural Loads (NPA). The latter showed that for the series of molecules studied, nitrogen atoms N_{26} and N_{28} are the privileged sites of electrophilic attack and the carbon atom C_{26} is the preferential site of nucleophilic attack.

References

[1] H. Abdelmadjid, «Synthèse des hétérocycles azotés à cinq chaînons dérivés de l'acide sorbique et détermination de leurs activités biologiques,» usto, 2013.

[2] N. A. Harry, S. Radhika, M. Neetha et G. and Anilkumar, «A novel catalyst-free mechanochemical protocol for the synthesis of 2,3-dihydro-1H-perimidines,» *J. Heterocycl. Chem.*, n° %13, p. 2–8, 2020.

[3] A. M. Giani, «Fluorescence studies on 2-(het)aryl perimidine derivatives,» *J. Lumin.*, vol. 179, p. 384–392, 2016.

[4] F. L. Hirshfeld, «"Bonded-atom fragments for describing molecular charge densities,",» *Theor. Chim. Acta,* vol. 44, n° %12, p. 129–138, 1977.

[5] A. Becke, «Density-functional thermochemistry III. The role of exact exchange,» *Journal of*

Chemistry Physical, vol. 98, n° %17, pp. 5648-5652, 1993.

[6] M. J. Frisch, G. W. Trucks, H. B. Schlegel et G. E. Scuseria, «Gaussian 09, Revision A.02,» Gaussian, Inc., Wallingford CT, 2009.

[7] B. G. Johnson, P. M. Gill et J. A. Pople, «The performance of a family of density functional methods,» *The Journal of Chemical Physics* , vol. 98, pp. 5612-5626, 1993.

[8] R. Hoffmann et R. Woodward, «The Conservation of Orbital Symmetry,» *J Am Chem Soc,* vol. 1, pp. 17-22, 1968.

[9] A. Bendjeddou, T. Abbaz, A. K. Gouasmia et D. Villemin, «Molecular Structure, HOMO-LUMO, MEP and Fukui Function Analysis of Some TTF-donor Substituted Molecules Using DFT (B3LYP) Calculations,» *International Research Journal of Pure & Applied Chemistry,* vol. 12, n° %11, 2016.

[10] J. S. N'dri, M.-R. Koné, C. G. Kodjo, A. L. C. kablan, S. T. Affi, L. Ouattara et N. Ziao, «Theoretical Study of the Chemical Reactivity of Five Schiff Bases Derived From Dapsone by the DFT Method,» *Chemical Science International Journal,* vol. 22, n° %14, pp. 1-11, 2018.

[11] T. Koopmans, «Úber die Zuordnung von Wellenfunktiomen und Eigenwerten zu den einzelnen Elektronen eines Atoms,» *Physica,* vol. 1, pp. 104-113, 1934.

[12] S. Dheivamalar, L. Sugi et K. Ambigai, «"Density Functional Theory Study of Exohedral Carbon Atoms Effect on Electrophilicity of Nicotine : Comparative Analysis,",» p. 17–31, January 2016.

[13] P. W. Ayers et R. G. Parr, «"Variational Principles for Describing Chemical Reactions: The Fukui Function and Chemical Hardness Revisited,",» *J. Am. Chem. Soc.,* vol. 122, n° %19, p. 2010–2018, Mars 2000.

[14] K. Fukui, T. Yonezawa et H. Shingu, «"A Molecular Orbital Theory of Reactivity in Aromatic Hydrocarbons,",» *J. Chem. Phys.,* vol. 20, n° %14, p. 722–725, April 1952.

[15] C. Morell, A. Grand et A. Toro-Labbé, «"Theoretical support for using the Δf(r) descriptor",» *Chem. Phys. Lett,* vol. 425, n° %14–6, p. 342–346, Juillet 2006.

[16] A. Mekky, H. Elhaes et M. El-Okr, «Molecular Electrostatic Potential Analysis of Nano-Scale Fullerene (C60) Crystals and Some Specific Derivatives: DFT Approach,» *J Nanomater Mol Nanotechnol* , vol. 4, 2015.