# Quantum computational calculations of novel *N*-sulfonylimine derivatives.

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**ABSTRACT**

A computer model based on the density functional theory (DFT) was developed for the identification of the physico-chemical parameters governing the bioactivity of novel *N*-sulfonylimine derivatives **1a-1f** containing a potential antibacterial pharmacophore sulfonamide unit. This study was performed using DFT / B3LYP with 6-31G (d, p) basis set. Information on the size, shape, charge density distribution, and site of chemical reactivity of molecules **1a-1f** was obtained by mapping the electron density isosurface with the electrostatic potential surface. The energies of frontier molecular orbitals and the LUMO-HOMO energy gap are measured to explain electronic transitions. To find the most reactive sites of the molecules studied, condensed Fukui functions were also calculated. The six compounds **1a-1f** analyzed here were previously synthesized by our group.

**Resumé**

Un modèle informatique basé sur la théorie fonctionnelle de la densité (DFT) a été développé pour l'identification des paramètres physico-chimiques régissant la bioactivité de nouveaux dérivés de *N*-sulfonylimine **1a-1f** contenant une pharmacophore antibacterien potential sulfonamide. Cette étude a été réalisée en utilisant la méthode DFT / B3LYP avec la base 6-31G (d, p). Des informations sur la taille, la forme, la distribution de densité de charge et le site de réactivité chimique des molécules **1a-1f** ont été obtenues en cartographiant l'isosurface de densité électronique avec la surface de potentiel électrostatique. Les énergies des orbitales moléculaires frontières et l'écart énergétique LUMO-HOMO sont mesurés pour expliquer les transitions électroniques. Pour trouver les sites les plus réactifs des molécules étudiées, des fonctions de Fukui condensées ont également été calculées. Les six composés **1a-1f** que nous avonts analysés ont été préalablement synthétisés par notre groupe.

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## 1. INTRODUCTION

*N*-sulfonylimines have attracted considerable attention from *organic* synthetic and medicinal *chemistry* communities, due to their efficient and strong reactivity, stability, and characteristics not found in other imine [1], they are considered as a special class of imine containing the sulfonyl moiety [2], the presence of this motif contributes to the activation of C = N bond in the molecule, which makes it possible to achieve excellent yields with the addition reaction [3]. *N*-sulfonylimines have been widely used in various transformations in organic synthesis in order to obtain *the* biologically active compounds [4].

In recent years, molecular modeling has become a very practical and powerful tool. It makes it possible to study and deal with chemical problems on a computer without going through experience. This approach uses theoretical computational methods to explain the problems of molecular structure and chemical reactivity [5].

DFT is a tool for describing chemical reactivity. Electronegativity and hardness are general characteristics of an atom, molecule or ion. To specify the reactivity of molecules, it is necessary to predict the electrophilic and nucleophilic sites. Recently, new theory-derived reactivity indices (DFTs) have emerged as powerful tools for predicting reactive sites of molecule systems [6-8].

Some parameters are already known such as electronic chemical potential ($\mu$) and electronegativity ($\chi$), and others are new such as electrophilia ($\omega$) and hardness ($\eta$), the latter were obtained from fundamental equations of DFT. Generally, these quantities express the response of the electron density of a molecule in an external field (V) and a number of electrons (N). They allow us to understand the behavior of a system in an overall way [9].

Fukui function (FF) provides information on the local site reactivity within the molecule and as such it provides a system for understanding of chemical reactions. These values correspond to thequalitative descriptors of reactivity of different atoms in the molecule. A study [10] has shown that FF is larger when attacked by soft reagents and in places where the FF is smaller when attacked by hard reagents.

The aim of our work is the theoretical study of reactivity and to determine energies, dipole moments and stability of six novel *N*-sulfonylimines (Fig.1) [11], using the density functional theory method (DFT) and To find out more reactive sites of the title molecules, condensed Fukui functions have been also calculated.

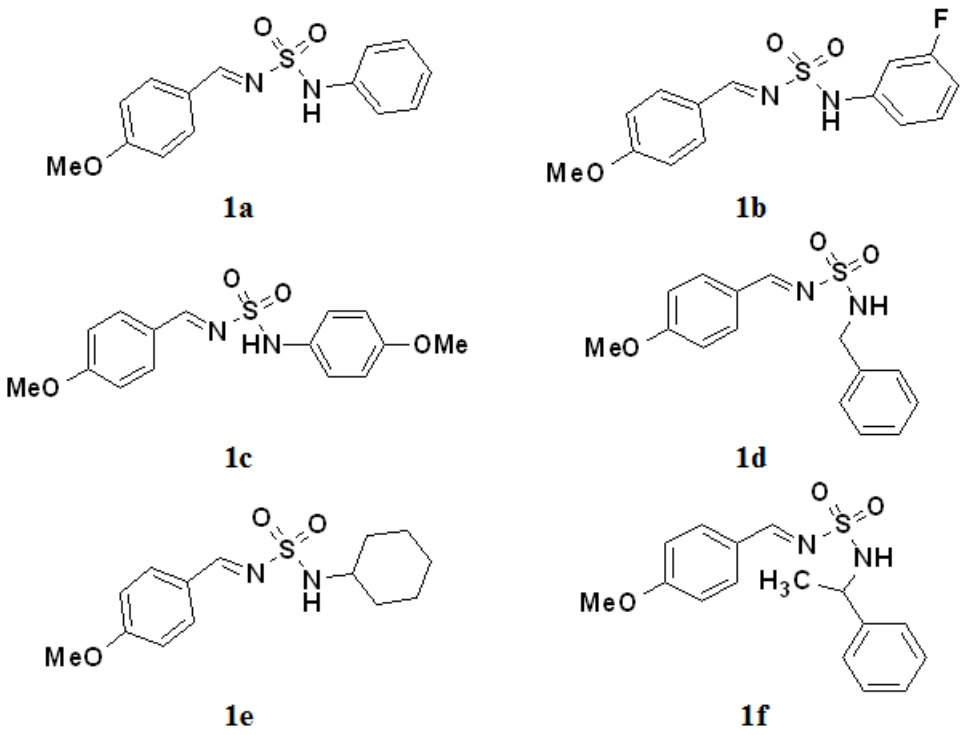


**Figure 1.** Structures of studied compounds.

## 2. RESEARCH METHOD

The density functional theory DFT/B3LYP with the 6-31 G (d, p) as basis set was adopted to calculate the properties of *N*-sulfonylimines a-f in the present work. The entire calculations were performed using Gaussian 09W program package [12].

## 3. RESULTS AND DISCUSSION

### 3.1. Molecular geometry:

The optimized molecular structures of title molecules obtained from Gauss view is shown in (Fig.2). The optimization geometrical parameters of *N*-sulfonylimines a-f obtained by B3LYP method with 6-31G (d,p) as basis set are listed in (Tab. 1-6). Alternate dispositions of sulfonylimine groups have been studied; C-C, N-C, N-S and S-O bonds, angles of groups and dihedral groups.

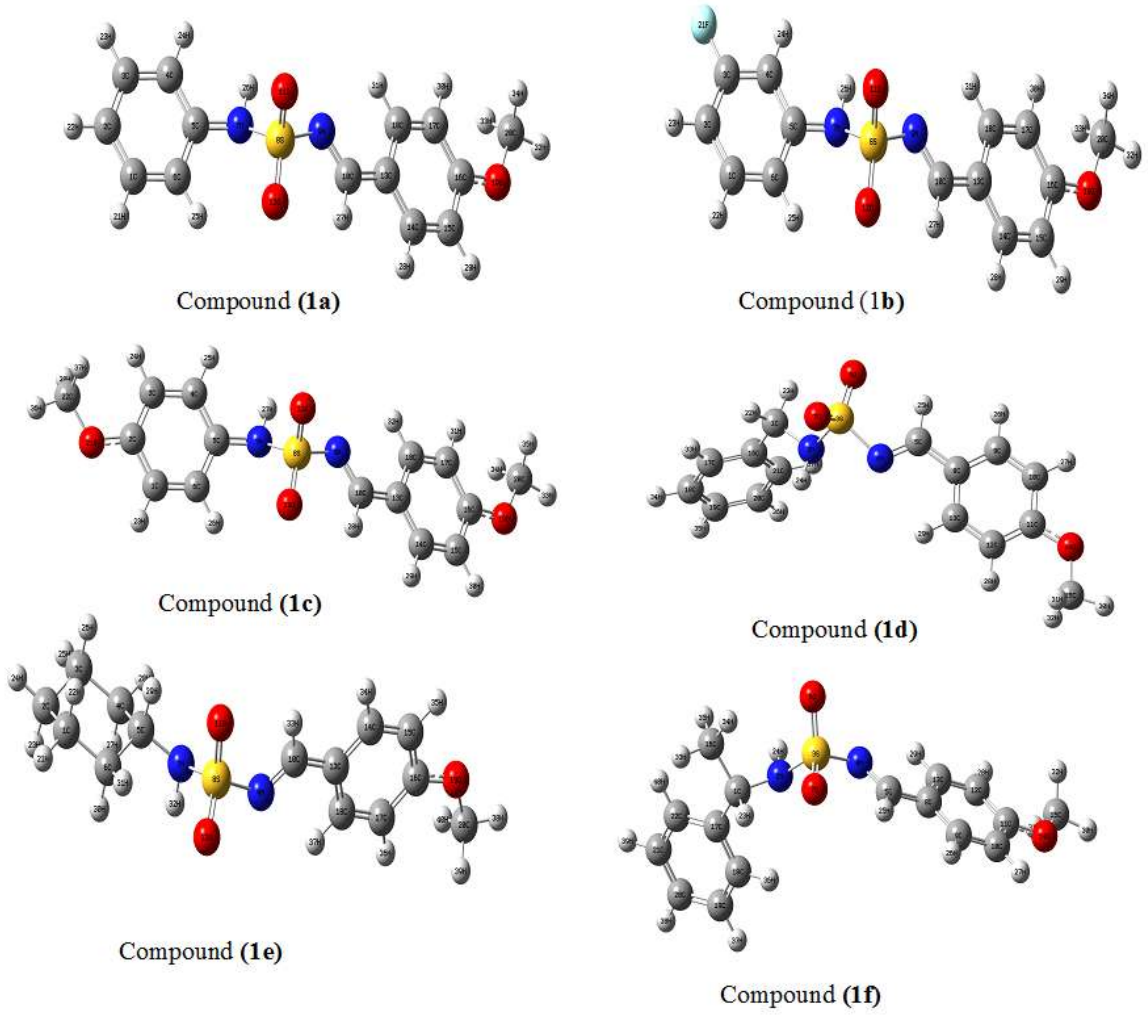


**Figure 2**. Optimized molecular structure of *N*-sulfonylimine **1a-1f.**

| Carbon | Hydrogen | Oxygen | Nitrogen | Fluorine | Sulfur |
|---|---|---|---|---|---|
| | | | | | |

**Table 1**. Optimized geometric parameters of compound **(1a)**

| **Bond Length(Å)** | | **Bond Angles (°)** | | **Dihedral Angles (°)** | |
|---|---|---|---|---|---|
| **(1,2)** | 1.3413 | **(2,1,6)** | 120.1635 | **(6,1,2,3)** | 0.2427 |
| **(1,6)** | 1.3425 | **(2,1,21)** | 119.8018 | **(6,1,2,22)** | 179.8925 |
| **(1,21)** | 1.1031 | **(1,2,3)** | 119.5786 | **(21,1,2,22)** | 0.2018 |
| **(2,22)** | 1.1027 | **(1,2,22)** | 120.2146 | **(1,2,3,4)** | -0.2423 |
| **(5,6)** | 1.3463 | **(3,4,5)** | 120.8735 | **(2,3,4,5)** | -0.3401 |
| **(5,7)** | 1.2732 | **(3,4,24)** | 118.3006 | **(2,3,4,24)** | 179.9224 |
| **(6,25)** | 1.1028 | **(4,5,6)** | 118.5152 | **(23,3,4,5)** | 179.7377 |
| **(7,8)** | 1.7012 | **(6,5,7)** | 123.4968 | **(3,4,5,7)** | 179.8644 |
| **(7,26)** | 1.0521 | **(5,7,8)** | 121.3324 | **(24,4,5,7)** | -0.4048 |
| **(8,9)** | 1.7073 | **(5,7,26)** | 110.876 | **(7,5,6,1)** | -179.8019 |
| **(8,11)** | 1.4567 | **(8,7,26)** | 114.8141 | **(7,5,6,25)** | -0.2845 |
| **(8,12)** | 1.4568 | **(7,8,9)** | 86.1605 | **(4,5,7,8)** | 136.041 |
| **(9,10)** | 1.2648 | **(7,8,11)** | 111.4828 | **(5,7,8,9)** | -159.9624 |
| **(10,13)** | 1.3477 | **(7,8,12)** | 112.2924 | **(5,7,8,11)** | -51.527 |
| **(10,27)** | 1.1046 | **(9,8,12)** | 108.1464 | **(5,7,8,12)** | 91.9875 |
| **(13,14)** | 1.3451 | **(11,8,12)** | 123.5947 | **(7,8,9,10)** | -179.5663 |
| **(14,28)** | 1.1038 | **(8,9,10)** | 123.2911 | **(11,8,9,10)** | 69.0483 |
| **(16,19)** | 1.3746 | **(9,10,13)** | 125.4545 | **(8,9,10,27)** | 0.1875 |
| **(19,20)** | 1.4088 | **(16,19,20)** | 118.771 | **(15,16,19,20)** | 179.6997 |
| **(20,34)** | 1.1129 | **(32,20,33)** | 108.1698 | **(16,19,20,34)** | 62.1884 |

**Table 2.** Optimized geometric parameters of compound **(1b)**

| **Bond Length(Å)** | | **Bond Angles (°)** | | **Dihedral Angles (°)** | |
|---|---|---|---|---|---|
| **(1,2)** | 1.3412 | **(1,2,3)** | 119.8703 | **(6,1,2,3)** | 0.1727 |
| **(1,22)** | 1.1031 | **(1,2,23)** | 120.0926 | **(6,1,2,21)** | 179.8212 |
| **(1,6)** | 1.3424 | **(2,1,22)** | 119.7925 | **(22,1,2,3)** | -179.4621 |
| **(2,23)** | 1.1026 | **(2,1,6)** | 120.1939 | **(23,2,3,21)** | 0.0135 |
| **(2,3)** | 1.3415 | **(2,3,4)** | 119.5397 | **(2,1,6,5)** | 0.3214 |
| **(5,6)** | 1.3461 | **(4,5,6)** | 118.3937 | **(2,1,6,25)** | -179.1492 |
| **(3,21)** | 1.3239 | **(5,6,25)** | 121.3117 | **(4,5,6,1)** | -0.8640 |
| **(5,7)** | 1.2734 | **(6,5,7)** | 123.6197 | **(4,5,6,25)** | 178.6438 |
| **(7,26)** | 1.0520 | **(4,5,7)** | 117.9783 | **(7,5,6,1)** | -179.7992 |
| **(7,8)** | 1.7021 | **(5,7,26)** | 111.0526 | **(7,5,6,25)** | -0.2930 |
| **(8,9)** | 1.7064 | **(8,7,26)** | 115.0598 | **(4,5,7,8)** | 137.059 |
| **(8,11)** | 1.4566 | **(7,8,9)** | 86.0522 | **(6,5,7,8)** | -43.9817 |
| **(9,10)** | 1.2647 | **(7,8,11)** | 110.0777 | **(5,7,8,11)** | -48.1746 |
| **(10,27)** | 1.1046 | **(7,8,12)** | 110.9513 | **(5,7,8,12)** | 92.4005 |
| **(10,13)** | 1.3476 | **(11,8,12)** | 123.6965 | **(26,7,8,11)** | 90.7224 |
| **(13,18)** | 1.3453 | **(9,8,12)** | 110.0608 | **(7,8,9,10)** | -178.8737 |
| **(18,31)** | 1.1035 | **(8,9,10)** | 123.2574 | **(12,8,9,10)** | -68.0249 |
| **(16,19)** | 1.3745 | **(9,10,13)** | 125.4472 | **(8,9,10,27)** | 0.1387 |
| **(19,20)** | 1.4089 | **(16,19,20)** | 118.7691 | **(17,16,19,20)** | -0.2872 |
| **(20,34)** | 1.1129 | **(19,20,34)** | 110.3502 | **(16,19,20,34)** | 62.2152 |

**Table 3.** Optimized geometric parameters of compound **(1c)**

| Bond Length(Å) | | Bond Angles (°) | | Dihedral Angles (°) | |
|---|---|---|---|---|---|
| **(1,2)** | 1.3471 | **(2,1,6)** | 122.8168 | **(6,1,2,3)** | 0.3257 |
| **(1,23)** | 1.1039 | **(2,1,23)** | 118.5942 | **(6,1,2,21)** | 179.9367 |
| **(2,21)** | 1.3746 | **(1,2,3)** | 115.7629 | **(23,1,2,3)** | -179.4232 |
| **(22,36)** | 1.1132 | **(1,2,21)** | 118.7236 | **(2,1,6,5)** | 0.2652 |
| **(22,38)** | 1.1129 | **(3,2,21)** | 125.5122 | **(1,2,21,22)** | -179.3515 |
| **(1,6)** | 1.3417 | **(2,21,22)** | 118.781 | **(4,5,7,8)** | 134.7532 |
| **(6,26)** | 1.1027 | **(36,22,37)** | 108.1641 | **(6,5,7,8)** | -46.3725 |
| **(5,6)** | 1.3438 | **(4,5,6)** | 117.6126 | **(5,7,8,9)** | -163.4849 |
| **(5,7)** | 1.2730 | **(5,7,8)** | 121.0594 | **(5,7,8,11)** | -55.1035 |
| **(7,27)** | 1.0522 | **(5,7,27)** | 110.6196 | **(5,7,8,12)** | 88.5875 |
| **(7,8)** | 1.7012 | **(7,8,9)** | 85.9044 | **(27,7,8,9)** | -26.9883 |
| **(8,9)** | 1.7075 | **(11,8,12)** | 123.6547 | **(27,7,8,11)** | 81.3931 |
| **(8,11)** | 1.4566 | **(7,8,11)** | 111.4225 | **(27,7,8,12)** | -134.9159 |
| **(8,12)** | 1.4567 | **(7,8,12)** | 112.4173 | **(11,8,9,10)** | 74.0354 |
| **(9,10)** | 1.2649 | **(9,8,11)** | 108.5959 | **(12,8,9,10)** | -62.4634 |
| **(10,13)** | 1.3476 | **(8,9,10)** | 123.329 | **(17,16,19,20)** | -0.0484 |
| **(10,28)** | 1.1046 | **(9,10,13)** | 125.4399 | **(16,19,20,35)** | 62.1098 |
| **(16,19)** | 1.3745 | **(9,10,28)** | 115.9799 | **(28,10,13,14)** | 0.0305 |
| **(19,20)** | 1.4089 | **(16,19,20)** | 118.7673 | **(2,21,22,36)** | 179.91 |
| **(20,33)** | 1.1131 | **(19,20,34)** | 110.352 | **(2,21,22,38)** | 61.9993 |

**Table 4.** Optimized geometric parameters of compound **(1d)**

| Bond Length(Å) | | Bond Angles (°) | | Dihedral Angles (°) | |
|---|---|---|---|---|---|
| **(1,2)** | 1.4611 | **(2,1,16)** | 108.3542 | **(16,1,2,3)** | -168.5951 |
| **(1,16)** | 1.5121 | **(2,1,22)** | 111.1401 | **(16,1,2,24)** | -45.3366 |
| **(1,23)** | 1.1149 | **(2,1,23)** | 110.4071 | **(22,1,2,24)** | 73.5616 |
| **(2,3)** | 1.706 | **(22,1,23)** | 107.3559 | **(23,1,2,3)** | 69.3224 |
| **(2,24)** | 1.0351 | **(1,2,3)** | 114.9113 | **(2,1,16,21)** | -106.8219 |
| **(3,4)** | 1.7055 | **(1,2,24)** | 107.8501 | **(1,2,3,4)** | -174.7993 |
| **(3,6)** | 1.4573 | **(3,2,24)** | 110.1412 | **(1,2,3,6)** | -62.7115 |
| **(3,7)** | 1.4572 | **(2,3,4)** | 84.4863 | **(1,2,3,7)** | 74.3845 |
| **(4,5)** | 1.2647 | **(2,3,6)** | 109.7042 | **(24,2,3,4)** | 63.1735 |
| **(5,8)** | 1.3478 | **(2,3,7)** | 107.7466 | **(24,2,3,6)** | 175.2613 |
| **(5,25)** | 1.1040 | **(4,3,6)** | 112.6293 | **(24,2,3,7)** | -47.6428 |
| **(8,9)** | 1.3452 | **(4,3,7)** | 111.4803 | **(2,3,4,5)** | 134.6444 |
| **(9,26)** | 1.1039 | **(6,3,7)** | 123.6431 | **(6,3,4,5)** | 25.5731 |
| **(16,21)** | 1.345 | **(3,4,5)** | 124.3194 | **(7,3,4,5)** | -118.4321 |
| **(17,33)** | 1.1028 | **(4,5,8)** | 125.3926 | **(3,4,5,8)** | 179.9061 |
| **(10,11)** | 1.3467 | **(4,5,25)** | 116.2134 | **(4,5,8,9)** | -179.9345 |
| **(11,14)** | 1.3745 | **(8,5,25)** | 118.3939 | **(10,11,14,15)** | -179.797 |
| **(14,15)** | 1.4088 | **(11,14,15)** | 118.7762 | **(11,14,15,30)** | 179.907 |
| **(15,30)** | 1.1132 | **(14,15,30)** | 107.7812 | **(17,16,21,20)** | 0.1296 |

**Table 5.** Optimized geometric parameters of compound **(1e)**

| Bond Length(Å) | | Bond Angles (°) | | Dihedral Angles (°) | |
|---|---|---|---|---|---|
| **(1,2)** | 1.5347 | **(2,1,6)** | 111.0774 | **(6,1,2,3)** | -56.428 |
| **(1,6)** | 1.5358 | **(2,1,22)** | 109.4345 | **(6,1,2,23)** | 64.3881 |
| **(1,21)** | 1.1164 | **(21,1,22)** | 107.0908 | **(21,1,2,23)** | -57.4061 |
| **(2,23)** | 1.1161 | **(4,5,6)** | 110.0239 | **(2,1,6,5)** | 56.5253 |
| **(5,6)** | 1.5394 | **(4,5,7)** | 108.3703 | **(3,4,5,6)** | 56.1541 |
| **(6,31)** | 1.1154 | **(5,7,8)** | 115.7024 | **(3,4,5,7)** | 178.817 |
| **(5,6)** | 1.5394 | **(5,7,32)** | 108.0798 | **(3,4,5,29)** | -63.0026 |
| **(5,29)** | 1.118 | **(8,7,32)** | 109.7052 | **(5,7,8,9)** | -167.8884 |
| **(5,7)** | 1.4668 | **(7,8,9)** | 85.8778 | **(5,7,8,11)** | -61.6669 |
| **(7,32)** | 1.0354 | **(7,8,11)** | 112.5247 | **(5,7,8,12)** | 85.1117 |
| **(7,8)** | 1.7030 | **(7,8,12)** | 114.0255 | **(32,7,8,9)** | -45.3253 |
| **(8,12)** | 1.4582 | **(9,8,11)** | 106.5536 | **(32,7,8,11)** | 60.8962 |
| **(8,9)** | 1.7085 | **(9,8,12)** | 107.1945 | **(32,7,8,12)** | -152.3252 |
| **(8,11)** | 1.4574 | **(11,8,12)** | 123.3551 | **(7,8,9,10)** | -164.8194 |
| **(9,10)** | 1.2647 | **(8,9,10)** | 123.7357 | **(8,9,10,13)** | -179.571 |
| **(10,33)** | 1.1046 | **(9,10,13)** | 125.4433 | **(8,9,10,33)** | 0.3068 |
| **(13,14)** | 1.3451 | **(9,10,33)** | 116.0341 | **(9,10,13,18)** | -0.105 |
| **(16,19)** | 1.3746 | **(16,19,20)** | 118.776 | **(16,19,20,40)** | 62.263 |
| **(19,20)** | 1.4088 | **(19,20,38)** | 107.7762 | **(16,19,20,38)** | -179.8302 |
| **(20,39)** | 1.1128 | **(38,20,39)** | 108.1727 | **(36,17,18,37)** | 0.0 |

**Table 6.** Optimized geometric parameters of compound **(1f)**

| Bond Length(Å) | | Bond Angles (°) | | Dihedral Angles (°) | |
|---|---|---|---|---|---|
| **(1,2)** | 1.4649 | **(2,1,16)** | 111.6176 | **(16,1,2,3)** | 70.9665 |
| **(1,16)** | 1.5382 | **(2,1,17)** | 108.6836 | **(16,1,2,24)** | -53.6058 |
| **(1,17)** | 1.5198 | **(2,1,23)** | 108.9806 | **(17,1,2,3)** | -167.7225 |
| **(1,23)** | 1.1180 | **(16,1,17)** | 109.8558 | **(17,1,2,24)** | 67.7052 |
| **(2,3)** | 1.6932 | **(16,1,23)** | 108.6047 | **(23,1,2,3)** | -48.9812 |
| **(2,24)** | 1.0344 | **(17,1,23)** | 109.06 | **(23,1,2,24)** | -173.5535 |
| **(3,4)** | 1.7099 | **(1,2,3)** | 116.1065 | **(17,1,16,34)** | 174.0909 |
| **(3,6)** | 1.4645 | **(1,2,24)** | 108.4858 | **(2,1,17,18)** | 126.3946 |
| **(3,7)** | 1.4643 | **(3,2,24)** | 110.1048 | **(1,2,3,4)** | 162.5763 |
| **(4,5)** | 1.2656 | **(2,3,4)** | 106.0968 | **(1,2,3,6)** | -95.5401 |
| **(5,25)** | 1.1044 | **(2,3,6)** | 115.0626 | **(1,2,3,7)** | 57.9492 |
| **(8,9)** | 1.3451 | **(2,3,7)** | 118.0093 | **(24,2,3,4)** | -73.6869 |
| **(8,13)** | 1.3452 | **(4,3,6)** | 93.5415 | **(2,3,4,5)** | -179.3489 |
| **(9,10)** | 1.3416 | **(4,3,7)** | 94.8187 | **(6,3,4,5)** | 63.29 |
| **(16,34)** | 1.1134 | **(6,3,7)** | 121.1125 | **(7,3,4,5)** | -58.3622 |
| **(17,18)** | 1.3459 | **(3,4,5)** | 125.2928 | **(3,4,5,8)** | -179.6897 |
| **(18,19)** | 1.3422 | **(4,5,8)** | 125.4313 | **(3,4,5,25)** | 0.1843 |
| **(19,20)** | 1.3411 | **(4,5,25)** | 116.2354 | **(5,8,13,12)** | 179.9325 |
| **(11,14)** | 1.3745 | **(8,5,25)** | 118.3332 | **(1,17,18,19)** | 179.9568 |
| **(14,15)** | 1.4089 | **(5,8,9)** | 120.5974 | **(1,17,18,36)** | 0.013 |

**3.2. Molecular electrostatic potential (MEPS)**

Molecular electrostatic potential (MEPS) at a point in space around a molecule gives information about the net electrostatic effect produced at that point by total charge distribution (electron + proton) of the molecule and correlates with dipole moments, electro-negativity, partial charges and chemical reactivity of the molecules. It provides a visual method to understand the relative polarity of the Molecules.

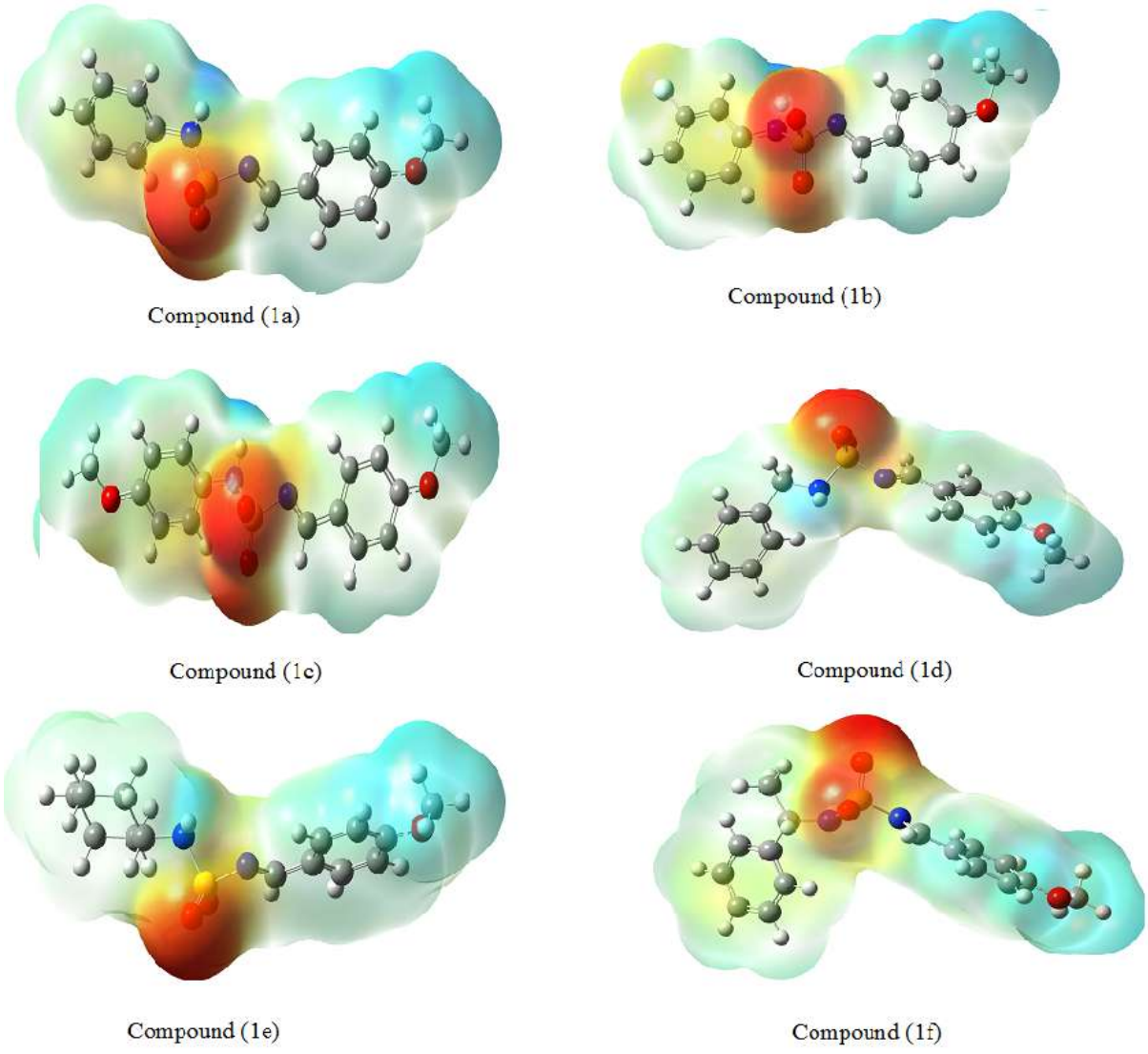


**Figure 3**. Molecular electrostatic potential surface of *N*-sulfonylimines **1a-1f**.

An electron density iso-surface mapped with electrostatic potential surface depicts the size, shape, charge density and site of chemical reactivity of the molecules. MEPS shown in (Fig. 3) calculated by DFT/B3LYP method with 6-31G (d, p) basis set is illustrates the charge distributions of the molecules three dimensionally.

As it can be seen from the (Fig. 3), the different values of the electrostatic potential at the surface are represented by different colors; red represents regions of most electronegative electrostatic potential,

blue represents regions of the most positive electrostatic potential and green represents regions of zero potential. Potential increases in the ordered, orange < yellow < green < blue. Blue indicates the strongest attraction and red indicates the strongest repulsion. Regions of negative potential are usually associated with the lone pair of electronegative atoms [13].

In all molecules, the regions exhibiting the negative electrostatic potential are localized near nitrogen, oxygen and sulfur atom of *N*-sulfonilimines group while the regions presenting the positive potential are localized vicinity of the hydrogen atoms of alkyl and aromatic cycled groups.

### 3.3. Frontier molecular orbitals (FMOs)

The frontier molecular orbital determine the way in which the molecule interacts with other species. HOMO (highest occupied molecular orbital), which can be thought the outermost orbital containing electrons, tends to give these electrons such as an electron donor. On the other hand, LUMO (lowest unoccupied molecular orbital) can be thought the innermost orbital containing free places to accept electrons [14].

Therefore, while the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. Energy difference between HOMO and LUMO orbital is called as energy gap that is an important stability for structures [15]. HOMO-LUMO helps to characterize the chemical reactivity and kinetic stability of the molecule [16]. A molecule with a small gap is more polarized and is known as soft molecule. Recently, the energy gap between HOMO and LUMO has been used to prove the bioactivity from intramolecular charge transfer (ICT) [17-18] because it is a measure of electron conductivity.

The HOMO energies, the LUMO energies and the energy gap for *N*-sulfonylimines **a-f** have been calculated using B3LYP level with6-31G (d, p) basis set. The pictorial representation of the HOMO and the LUMO for compounds is shown in (Fig. 4), and the difference in Gap energies when 1a has the lowest energy however 1b has the highest energy which give an idea for the reactivity of the molecules.

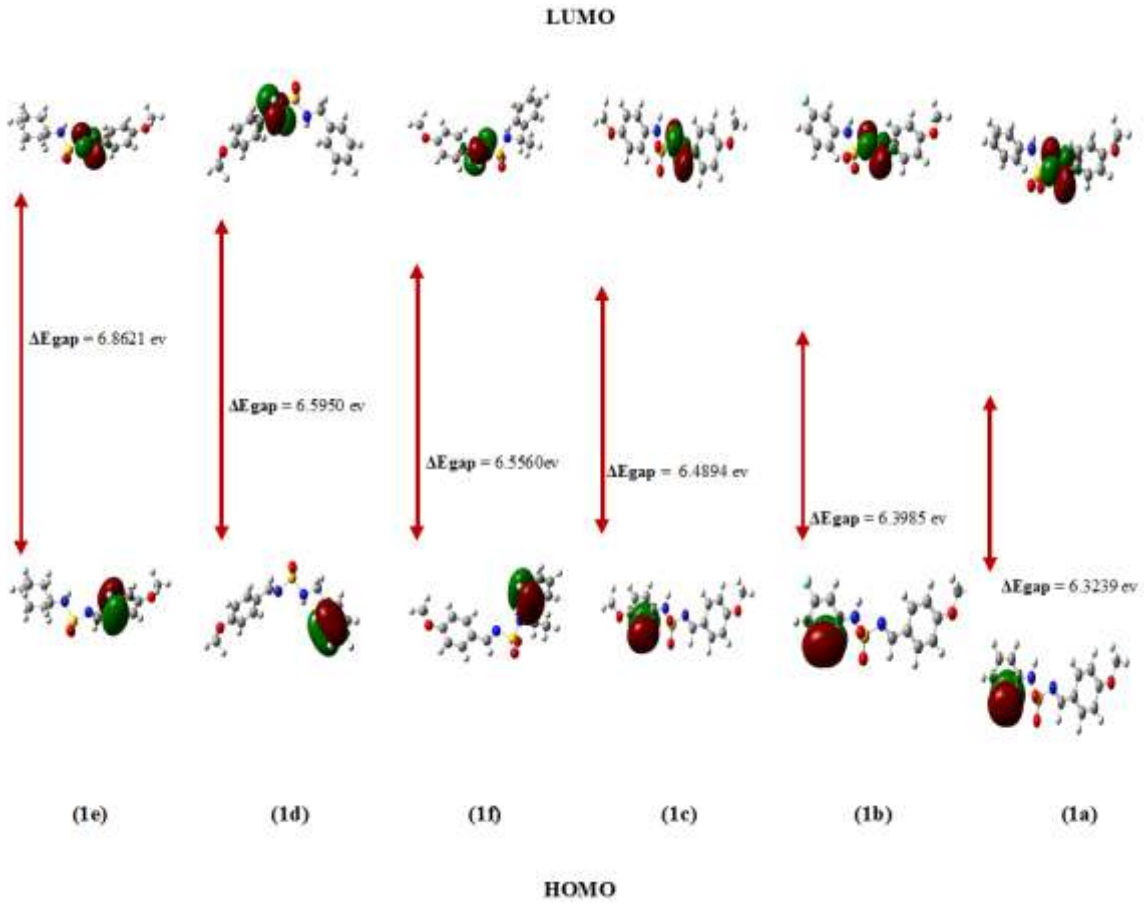


**Figure 4.** HOMO-LUMO Structure with the energy level diagram of compounds **1a-1f**.

### 3.4. Global reactivity descriptors

The chemical reactivity of the molecular systems has been determined by the conceptual density functional theory DFT [19]. Electronegativity (χ) chemical potential (μ), global hardness (η), global softness (S) and electrophilicity index (w) are global reactivity descriptors, highly successful in predicting global reactivity trends on the basis of Koopmans's theorem, [20] global reactivity descriptors of *N*-sulofnylimines are calculated using the energies of frontier molecular orbitals $E_{HOMO}$, $E_{LUMO}$ as :

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

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

$\eta = 1/2(E_{LUMO} - E_{HOMO})$ (3)

$S = 1/\eta$ (4)

$\omega = \mu^2 /2\eta$ (5)

$I = -E_{HOMO}$ and $A = -E_{LUMO}$ (6)

Where I and A are the ionization potential and electron affinity of the compounds, respectively. The energies of frontier molecular orbitals ($E_{LUMO}$, $E_{HOMO}$) reactivity descriptors for molecules a-f are listed in (Tab. 7), All the calculated values are obtained by B3LYP/6-31G (d, p).

**Table 7.** Quantum chemical descriptors of *N*-sulfonylimines **a-f.**

| **Descriptors** | **Phase gazeuse** | | | | | |
|---|---|---|---|---|---|---|
| **Moleculaire** | **1a** | **1b** | **1c** | **1d** | **1e** | **1f** |
| **Log P** | 2.84 | 3.00 | 2.71 | 3.15 | 3.85 | 3.46 |
| **$\alpha_{Tot}$ (Bohr$^3$)** | 205.42 | 206.52 | 225.33 | 211.88 | 205.10 | 222.42 |
| **μ (D)** | 6.5037 | 7.0612 | 5.9598 | 6.0645 | 5.8576 | 5.7232 |
| **$E_{HOMO}$ (eV)** | -6.4621 | -6.6458 | -6.5236 | -6.5963 | -6.8893 | -6.5231 |
| **$E_{LUMO}$ (eV)** | -0.1382 | -0.2473 | -0.0342 | -0.0013 | -0.0272 | 0.0329 |
| **ΔEgap(eV)** | 6.3239 | 6.3985 | 6.4894 | 6.5950 | 6.8621 | 6.5560 |
| **E (u.a)** | -1275.2173 | -1374.4489 | -1389.7415 | -1314.5327 | -1278.8543 | -1353.8497 |
| **I (eV)** | 0.1382 | 0.2473 | 0.0342 | 0.0013 | 0.0272 | 0.0329 |
| **A (eV)** | 6.4621 | 6.6458 | 6.5236 | 6.5963 | 6.8893 | 6.5231 |
| **(η)** | **3.1619** | 3.1992 | 3.2447 | 3.2975 | 3.4310 | 3.2780 |
| **(*S*)** | 0.3162 | 0.3125 | 0.3081 | 0.3032 | 0.2914 | 0.3050 |
| **(μ)** | -3.3001 | -3.4465 | -3.2789 | -3.2988 | -3.4582 | -3.2451 |
| **(χ)** | 3.3001 | 3.4465 | 3.2789 | 3.2988 | 3.4582 | 3.2451 |
| **(ω)** | 1.7222 | 1.8565 | 1.6567 | 1.6500 | 1.7428 | 1.6062 |

$E_{HOMO}$: Energy of highest occupied molecular orbital, $E_{LUMO}$: Energy oflowest unoccupied molecular orbital, ΔEgap: Energetic gap, I: Ionization potential, A: Electron affinity, μ: Chemical potential, χ: Electronegativity; η: Hardness, S: Softness, ω: Electrophilicity index.

As presented in (Tab.7), the compound which have the lowest energetic gap is the compound a (ΔEgap = 6.3239 eV). This lower gap allows it to be the softest molecule. The compound that have the highest energy gap is the compound **1e** (ΔEgap = 6.8621 eV). The compound that has the highest HOMO energy is the compound **1a** ($E_{HOMO}$ = -6.4621 eV). This higher energy allows it to be the best electron donor.

The compound that has the lowest LUMO energy is the compound **1a** ($E_{LUMO}$ = -0.2473 eV) which means that it can be the best electron acceptor. The two properties like I (potential ionization) and A (affinity) are so important, the determination of these two properties allow us to calculate the absolute electronegativity (χ) and the absolute hardness (η). These two parameters are related to the one-electron orbital energies of the HOMO and LUMO respectively. The chemical reactivity varies with the structural of molecules. Chemical hardness (softness) value of compound **1a** (η = 3.1619 eV, S = 0.3162 eV) is lesser (greater) among all the molecules.

Thus, compound **1e** is found to be more reactive than all the compounds. Compound **1e** possesses higher electronegativity value (χ = 3.4582 eV) than all compounds so; it is the best electron donnor. The value of ω for compound **1f** (ω = 1.6062 eV) indicates that it is the stronger electrophiles than all compounds. Compound **1f** has the smaller frontier orbital gap so, it is more polarizable and is associated with a high chemical reactivity, low kinetic stability and is also termed as soft molecule.

### 3.5. Local reactivity descriptors

The local reactivity descriptor like Fukui function indicates preferred regions where a chemical specie (molecule) will amend its density when numbers of electrons are modified or it indicates tendency of electronic density to deform at a given position upon accepting or donating electrons [21].

The condensed or atomic Fukui functions on the k$^{th}$ atom site, for electrophilic ($f^{+}_{k}$), nucleophilic ($f^{-}_{k}$) and free radical ($f^{0}_{k}$) attacks are defined as:

For nucleophilic attack $f^{-}_{k} = [q_k(N+1) - q_k(N)]$

For electrophilic attack $f^{+}_{k} = [q_k(N) - q_k(N-1)]$

For radical attack $f^{0}_{k} = [q_k(N+1) - q_k(N-1)]$

Where $q$ (N), $q$ (N+1), and $q$ (N-1) are the electronic population of the atom k in neutral, cationic and anionic systems respectively [22]. The reactive sites on *N*-sulfonylimines **1a-f** are calculated by the DFT/B3LYP method with 6-31G (d,p) basis set and shown in (Tab. 8-13). All calculations have been realised by UCA Fukui.

**$f^{+}$:** Fukui functions for nucleophilic attack, $f^{-}$: Fukui functions for electrophilic attack, $f^{0}$: Fukui functions for radical attack.

**Table 8**. Order of the reactive sites on compounds **1a.**

| **Compound (1a)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Atom** | **5 C** | **7 N** | **8 S** | **9 N** | **10 C** | **11 O** | **12 O** | **13 C** | **18 C** |
| $f^{+}$ | 0.0007 | 0.0005 | 0.0038 | 0.3906 | 0.5943 | 0.0002 | 0.0001 | 0.0094 | 0.0001 |
| **Atom** | **1 C** | **2 C** | **5 C** | **6 C** | **7 N** | **8 S** | **10 C** | **-** | **-** |
| $f^{-}$ | 0.4769 | 0.0135 | 0.0151 | 0.4940 | 0.0001 | 0.0001 | 0.0001 | - | - |
| **Atom** | **1 C** | **2 C** | **5 C** | **6 C** | **7 N** | **8 S** | **9 N** | **10 C** | **14 C** |
| $f^{0}$ | 0.2385 | 0.0067 | 0.0079 | 0.2470 | 0.0003 | 0.0019 | 0.1953 | 0.2972 | 0.0047 |

**Table 9**. Order of the reactive sites on compounds **1b**.

| **Compound (1b)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Atom** | **5 C** | **7 N** | **8 S** | **9 N** | **10 C** | **11 O** | **12 O** | **13 C** | **18 C** |
| $f^{+}$ | 0.0007 | 0.0005 | 0.0039 | 0.3888 | 0.5959 | 0.0002 | 0.0001 | 0.0094 | 0.0001 |
| **Atom** | **1 C** | **2 C** | **4 C** | **5 C** | **6 C** | **7 N** | **8 S** | **-** | **-** |
| $f^{-}$ | 0.4580 | 0.0126 | 0.0001 | 0.0157 | 0.5132 | 0.0001 | 0.0001 | - | - |
| **Atom** | **1 C** | **2 C** | **5 C** | **6 C** | **7 C** | **8 S** | **9 N** | **10 C** | **13 C** |
| $f^{0}$ | 0.2290 | 0.0063 | 0.0082 | 0.2566 | 0.0003 | 0.0020 | 0.1944 | 0.2980 | 0.0047 |

**Table 10**. Order of the reactive sites on compounds **1c**.

| **Compound (1c)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Atom** | **5 C** | **7 N** | **8 S** | **9 N** | **10 C** | **11 O** | **12 O** | **13 C** | **18 C** |
| $f^{+}$ | 0.0006 | 0.0005 | 0.0036 | 0.3926 | 0.5927 | 0.0002 | 0.0001 | 0.0093 | 0.0001 |
| **Atom** | **1 C** | **2 C** | **5 C** | **6 C** | **7 N** | **8 S** | **12 O** | **21 O** | **-** |
| $f^{-}$ | 0.5097 | 0.0146 | 0.0139 | 0.4614 | 0.0001 | 0.0001 | 0.0001 | 0.0001 | - |
| **Atom** | **1 C** | **2 C** | **5 C** | **6 C** | **7 N** | **8 S** | **9 N** | **10 C** | **13 C** |
| $f^{0}$ | 0.2548 | 0.0073 | 0.0072 | 0.2307 | 0.0003 | 0.0019 | 0.1963 | 0.2964 | 0.0046 |

**Table 11**. Order of the reactive sites on compounds **1d**.

| **Compound (1d)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Atom** | **1 C** | **2 N** | **3 S** | **4 N** | **5 C** | **6 O** | **7 O** | **8 C** | **10 C** |
| $f^{+}$ | 0.0003 | 0.0004 | 0.0034 | 0.3940 | 0.5918 | 0.0001 | 0.0002 | 0.0093 | 0.0001 |
| **Atom** | **1 C** | **2 N** | **14 O** | **17 C** | **18 C** | **19 C** | **35 H** | **-** | **-** |
| $f^{-}$ | 0.0001 | 0.0001 | 0.0144 | 0.0138 | 0.4894 | 0.4796 | 0.0024 | - | - |
| **Atom** | **1 C** | **3 S** | **4 N** | **5 C** | **8 C** | **16 C** | **19 C** | **20 C** | **21 C** |
| $f^{0}$ | 0.0002 | 0.0017 | 0.1970 | 0.2959 | 0.0046 | 0.0072 | 0.0069 | 0.2447 | 0.2398 |

**Table 12**. Order of the reactive sites on compounds **1e**.

| **Compound (1e)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Atom** | **4 C** | **5 C** | **7 N** | **8 S** | **9 N** | **10 C** | **11 O** | **12 O** | **13 C** |
| $f^+$ | 0.0001 | 0.0005 | 0.0005 | 0.0034 | 0.3965 | 0.5891 | 0.0001 | 0.0002 | 0.0092 |
| **Atom** | **7 N** | **8 S** | **10 C** | **13 C** | **14 C** | **17 C** | **18 C** | **-** | **-** |
| $f^-$ | 0.0001 | 0.0002 | 0.0095 | 0.5575 | 0.0123 | 0.0121 | 0.4076 | - | - |
| **Atom** | **5 C** | **7 N** | **8 S** | **9 N** | **10 C** | **13 C** | **14 C** | **18 C** | **40 H** |
| $f^0$ | 0.0003 | 0.0003 | 0.0018 | 0.1983 | 0.2993 | 0.2833 | 0.0061 | 0.2039 | 0.0003 |

**Table 13**. Order of the reactive sites on compounds **1f**.

| **Compound (1f)** | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **Atom** | **5 C** | **7 O** | **8 C** | **9 C** | **10 C** | **11 C** | **12 C** | **13 C** | **18 C** |
| $f^+$ | 0.0007 | 0.0005 | 0.0039 | 0.3888 | 0.5959 | 0.0002 | 0.0001 | 0.0094 | 0.0001 |
| **Atom** | **1 C** | **2 N** | **5 C** | **7 O** | **8 O** | **-** | **-** | **-** | **-** |
| $f^-$ | 0.4580 | 0.0126 | 0.0157 | 0.5132 | 0.0001 | - | - | - | - |
| **Atom** | **1 C** | **2 N** | **5 C** | **6 O** | **8 C** | **9 C** | **10 C** | **13 C** | **-** |
| $f^0$ | 0.2290 | 0.0063 | 0.0082 | 0.2566 | 0.0020 | 0.1944 | 0.2980 | 0.0047 | - |

From the tables 8-13, the parameters of local reactivity descriptors show that 10C and 9N are the more reactive sites in compounds **1a, 1b, 1c, 1d** and **e;** for the compound **1f** are10C and 9C for nucleophilic attacks. The more reactive sites in radical attacks are 1C, 6C and 10C for compounds 1**a, 1b, 1c** however 5C, 10C for the compound **1d**, 10C, 13C and 18C for the compound **e**, and 1C, 5O, 9C, 10C for the compound **1f**. The more reactive sites for electrophilic attacks are 1C, 6C for compounds 1**a, 1b, 1c** respectively and 18C, 19C for the compound **1d**, 13C,18C for the compound **e**, and 1C, 7O for the compound **1f.**

## 4. CONCLUSION

This work reports the computational analysis of new series of *N*-sulfonylimine derivatives. The geometry of all synthesized compounds was optimized with DFT/B3LYP methods using 6-31G (d, p) basis to determine tasks that coordinate electron density with energy. The molecular structural parameters of studied molecules have been computed in this work by using the same method cited above. The MEP map shows the negative potential sites are on sulfamide function as well as the positive potential sites around the hydrogen atoms. Our findings reveal that all synthesized compounds **1a-1f,** In addition, theoretical results from reactivity descriptors for title compounds show most reactivity at 10 C and 9 N for nucleophilic attack.

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