Theoretical Study for Chemical Reactivity Descriptors of Tetrathiafulvalene in gas phase and solvent phases based on Density Functional Theory

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1. Introduction

Tetrathiafulvalene (TTF) is a type of organic semiconductor that has attracted a lot of attention in recent years as potential charge transfer material in organic electronic systems. It contains 14 atoms and 104 electrons; however, it has a higher capacity for donating electrons. TTFs were produced and widely used as electron donors to generate charge transfer complexes in the creation of organic conductors and supramolecular chemistry [1-3].

Many experts from biology, pharmacology, and chemistry have worked on the TTF in recent years, revealing information about this chemical and its derivatives. Tahar Abbaz et.al. studied the reactivity of tetrathiafulvalene with derivatives and focused on molecular structure and chemical reactivity of some p-nitrophenyl Tetrathiafulvalene [4]. D. Jerroundi, et.al calculated the quantum chemistry calculation parameters of TTF and derivatives [5]. Hendrik, et.al. investigated how to control motion in mechanically interlocked molecules [6]. Huixin, et.al. explored the interactions between tetrathiafulvalene units in dimeric structures [7]. P. Gnanamozhi, at.al. dealt with the structure and FMOs gap of Tetrathiafulvalene (TTF) as organic superconductors [8].

In the recent years, the Density Functional Theory (DFT), has been the most common quantum chemical method used for calculating different molecular properties such as physical, chemical and biological systems [9, 10]. Chemical descriptors were described by DFT for studying and forecasting reactivity indices and selectivity [11-18].

The objective of this study is to analyze Frontier Molecular Orbital (FMOs) energies and obtain global reactivity descriptors. Moreover, Mulliken population analysis and Fukui Functions (FFs) were calculated to determine the atomic charge...
distribution for selecting electrophile and nucleophile areas of the TTF compound using DFT with a basis set (B3LYP/6-311++G).

2. Materials and Methods

The optimized structure of TTF was performed on personal computer using the Gaussian 09W software packages developed by Frisch and coworkers. Gaussian output files were visualized by means of Gaussian View 06 programme. The theoretical calculations were performed to investigate the geometric parameters and electronic properties of this compound such as ionization potential (I), electron affinity (A), lowest unoccupied molecular orbital (E_LUMO), highest occupied molecular orbital (E_HOMO), and energy gap (E_Δ). Koopman’s theorem for closed-shell molecules can be used to compute the various global chemical reactivity descriptors in different types of solvents. Mulliken population analysis, Fukui functions, and thermodynamic parameters can be computed and discussed [19-26].

3. Results and Discussion

3.1. Global Reactivity Descriptors and Dipole Moment

The molecular structures of TTF compound were optimized using the quantum mechanical method at the B3LYP/6-311++G basis set in gas phase and in solvents. The global chemical reactivity descriptors in (Table 1 and Table 2) such as ionization potential (I), electron affinity (A), lowest unoccupied molecular orbital (E_LUMO), highest occupied molecular orbital (E_HOMO), and energy gap (E_Δ). Koopman’s theorem for closed-shell molecules can be used to compute the various global chemical reactivity descriptors in different types of solvents. Mulliken population analysis, Fukui functions, and thermodynamic parameters can be computed and discussed [19-26].

The global chemical reactivity descriptors such as hardness (η), softness (S), electronegativity (χ), chemical potential (μ), electrophilicity index (ω), nucleofugality (ΔE_n), electrophilicity (ΔE_e) could be calculated from HOMO and LUMO energy orbitals achieved in the gas phase and solvents phase by using density functional theory with B3LYP/6-311++G basis set of TTF molecular structure as shown in Figure 1.

![Figure 1: Optimized structure of TTF compound](image)

One of the main components in this study is the effect of solvents, which determines the rate of chemical reaction dependent on polarity. The chemical structure of this substance is related to changes in the values of global chemical reactivity characteristics in the solvent phases. The electronic affinity (A) is a measure of the capacity of the compound to gain valence electrons, while ionization potential (I) is a measure of the ability of the compound to lose electrons. The higher value of ionization potential energy(I) parameter indicates that it is difficult to eliminate an electron to form an ion, whereas a molecule with a high value of electron affinity (A) signifies that it is difficult to add electron. As can be seen in Table 1, it is difficult to remove an electron from the gas phase to the solvent phase to form an ion as a result of the higher value of ionization potential. On the other hand, the smaller the electron affinity, the simpler it is to add an electron to create an ion.

Water and several polar solvents are incapable to create significant attractive interactions with non-polar molecules because the hydrogen and carbon atoms are well bonded together through non-polar Vander Waals interactions.

The frontier energy gap, E_HOMO, and E_LUMO energy of TTF in the gas phase and solvents phase are determined by density functional theory with the basis set (B3LYP/6-311++G). The HOMO-LUMO gap is strongly related to the optical and electronic properties of TTF. The HOMO energy denotes the ability to give electrons, whereas the LUMO energy denotes the ability to receive electrons. The energy gap between HOMO-LUMO orbitals characterizes molecular chemical stability, optical polarizability, and chemical reactivity. The smaller the energy gap (soft) between LUMO and HOMO energy orbitals, the easier it is for the HOMO electron to be transferred to an excited state (LUMO). The wider the energy gap, the more difficult it is for the (HOMO) to donate an electron to the excited state (LUMO). TTF has a lower energy gap in CCl_4 (3.899 eV) than gas phase and other solvents.

Consequently, the electron transfer from HOMO to LUMO of the molecule in CCl_4 is comparatively easier than that in the gas phase and other solvent phases. TTF has a greater bandgap energy in water (3.984 eV) than in the gas phase and the rest of the solvent phases, as indicated in Table 2. Therefore, the electron transfer from HOMO to LUMO of the molecule in water is
relatively harder than that in the gas phase. The bandgap energy of
this compound in the gas phase is 3.872 eV, and this result is
an agreement with the calculated values in [31, 32]. As seen in Table
1, the electron jumps from the HOMO to the LUMO energy
orbital more easily (softer) in the gas phase than in the other
solvent phases combined.

Table 1: Ionization energy, potential energy, HOMO, LUMO, and energy gap of TTF in the gas phase and diverse solvents

| Tetrathiafulvalene (C₅H₄S₄) | Calculations |
|-----------------------------|-------------|
|                             | Gas phase | Water | Acetone | THF | CCl₄ | Benzene |
| IP (eV)                     | 5.109     | 5.263 | 5.250   | 5.222 | 5.159 | 5.155   |
| EA (eV)                     | 1.237     | 1.317 | 1.308   | 1.291 | 1.260 | 1.255   |
| E_HOMO (eV)                 | -5.109    | -5.263| -5.250  | -5.222| -5.159| -5.155  |
| E_LUMO (eV)                 | -1.237    | -1.317| -1.308  | -1.291| -1.260| -1.255  |
| E_r (eV)                    | 3.872     | 3.946 | 3.942   | 3.931 | 3.899 | 3.900   |

Electronegativity and the electronic chemical potential are
important parameters in the quantum chemical reaction. The
more the value of electronegativity, the greater the capability of
atoms or molecules to attract electrons, whereas the greater the
value of chemical potential value, the more the reactivity and less
stability. This molecule in water has a higher electronegativity
than other solvents as shown in Table 2. TTF has the maximum
chemical potential in the gas phase and benzene solvent. As a
result, this molecule is more reactive and less stable in both gas
phase and benzene solvent, as seen in Table 2. The electrophilicity
index magnitude is used as a chemical structural
descriptor for the examination of the chemical reactivity of
molecules. More reactive nucleophile is considered to have a
lower value of (ω) than a strong electrophile with a high value of
(ω). As shown in Table 2, TTF in benzene solvent is a more
reactive nucleophile, indicating that this molecule is a good
electrophile when compared to water solvent. Electrofugality and
nucleofugality are important concepts to describe the chemical
reaction. Due to the greater polarity of water compared to the gas
phase and the other solvents, TTF in water has the highest
electrofugality and nucleofugality.

Table 2: Global chemical reactivity descriptors of TTF in the gas phase and different types of solvent

| Tetrathiafulvalene (C₅H₄S₄) | Calculations |
|-----------------------------|-------------|
|                             | Gas phase | Water | Acetone | THF | CCl₄ | Benzene |
| η (eV)                      | 1.936     | 1.973 | 1.971   | 1.966 | 1.949 | 1.950   |
| S(eV)^{-1}                  | 0.258     | 0.253 | 0.254   | 0.254 | 0.257 | 0.256   |
| χ (eV)                      | 3.173     | 3.290 | 3.279   | 3.255 | 3.210 | 3.205   |
| μ (eV)                      | -3.173    | -3.290| -3.279  | -3.255| -3.210| -3.205  |
| ω (eV)                      | 2.600     | 2.743 | 2.725   | 2.742 | 2.710 | 2.703   |
| ΔE_r (eV)                   | 0.395     | 0.440 | 0.434   | 0.423 | 0.409 | 0.404   |
| ΔE_r (eV)                   | 6.741     | 7.020 | 6.992   | 6.934 | 6.826 | 6.814   |

The dipole moment parameter is expressed in Debye (D) unit.
The stronger the intermolecular interactions, the bigger the
magnitude of the dipole moment. Similarly, the larger the
charge on the C₅H₄S₄ compound is negative (1C, 2C, 3C, 4C, 5C,
6C) and positive (7S, 8S, 9S, 10S), with the full atomic charge on
hydrogen atoms being positive. As shown in Table 4, the
existence of substantial negative atomic charges on (1C and 2C)
in the gas phase and solvent mediums such as benzene and CCl₄
indicates that these carbons have the largest electron density and
can easily interact with the positively charged region of the
receptor.

Table 3: Effects of solvent polarity on the value of dipole moment of TTF

| Dipole moment (Debye) | Gas phase | Water | Acetone | THF | Benzene | CCl₄ |
|-----------------------|-----------|-------|--------|-----|---------|------|
| X                     | 0.000     | 0.000 | 0.000  | 0.000| 0.000   | 0.000|
| Y                     | 0.000     | 0.000 | 0.000  | 0.000| 0.000   | 0.000|
| Z                     | 0.000     | 0.000 | 0.000  | 0.000| 0.000   | 0.000|
| Total                 | 0.000     | 0.000 | 0.000  | 0.000| 0.000   | 0.000|

3.2. Mulliken Population Analysis and Fukui Functions

The calculation of the Mulliken atomic charge is essential in the
application of the molecular system for quantum chemical
computation. The Mulliken population analysis influences
several molecule attributes, such as dipole moment, electronic
structure, and other chemical system properties. The distribution
of positive and negative charges has a significant impact on the
length of the connection between the atoms [35,36]. The atomic
charge of positive atoms is important in describing the molecular
structure and the interactions between the molecules. A positive
charge on atoms or molecules indicates a lower electron density,
which makes them less reactive. On the other hand, negative
charges enhance the electron density, making the atoms more
reactive. The distribution of charges in a molecule can be
quantitatively analyzed using Mulliken population analysis, which
provides valuable information about the molecular structure and
reactivity.
The FFs of the system depicts the more reactive locations of this chemical, and these equations (9-14) use the Mulliken population to assess Fukui functions[30].

\[
f_k^+ = q(N+1) - q(N) \quad \text{..........................(9)}
\]

\[
f_k^- = q(N) - q(N-1) \quad \text{..........................(10)}
\]

\[
f_k^0 = \frac{q(N+1) - q(N-1)}{2} \quad \text{..........................(11)}
\]

Where, \(f_k^+\) is a nucleophilic attack, \(f_k^-\) the electrophilic attack, and \(f_k^0\) is a radical attack.

The nucleophilicity and electrophilicity were proposed by Morrel et al[30] and can be explained by the dual descriptor (\(\Delta f(r)\)).

\[
\Delta f(r) = f_k^+ - f_k^- \quad \text{..........................(12)}
\]

If \(\Delta f(r) < 0\), then the site is electrophile attack and if \(\Delta f(r) > 0\) then the site is a nucleophile attack. On the other hand, local softness \((S_k^+, S_k^-, S_k^0)\) and local electrophilicity indices \((\omega_k^+, \omega_k^-, \omega_k^0)\) can be calculated by the following equations:

\[
S_k^+ = S f_k^+ , S_k^- = S f_k^- , S_k^0 = S f_k^0 \quad \text{..........................(13)}
\]

\[
\omega_k^+ = \omega f_k^+ , \omega_k^- = \omega f_k^- , \omega_k^0 = \omega f_k^0 \quad \text{..........................(14)}
\]

Where, +, - and 0 are design nucleophilic, electrophilic, and radical attack, respectively.

If \(\Delta f(r) < 0\), then the site is electrophile attack and on the contrary if \(\Delta f(r) > 0\), then the site is a nucleophile attack. The atomic charges on (1 C, 2 C, 11 H, 12 H, 13 H, 14 H) are electrophile attack while the atomic charges on (3 C, 4 C, 5 C, 6 C, 7 S, 8 S, 9 S, 10 S) are nucleophile attack. The maximum value on 7 S, 8 S, 9 S, 10 S specifies that higher radical attack compared to other atoms as shown in Table 5.

### Table 5: Fukui Functions for TTF from the NBO charges

| Atoms | q(N) | q(N-1) | q(N+1) | \(f_k^+\) | \(f_k^-\) | \(f_k^0\) | \(f_r\) |
|-------|------|--------|--------|----------|----------|----------|--------|
| 1 C   | -0.396 | -0.412 | -0.404 | -0.008   | 0.016    | 0.004    | -0.024 |
| 2 C   | -0.396 | -0.412 | -0.404 | -0.008   | 0.016    | 0.004    | -0.024 |
| 3 C   | -0.400 | -0.416 | -0.374 | 0.026    | 0.016    | 0.021    | 0.01   |
| 4 C   | -0.400 | -0.416 | -0.374 | 0.026    | 0.016    | 0.021    | 0.01   |
| 5 C   | -0.400 | -0.416 | -0.374 | 0.026    | 0.016    | 0.021    | 0.01   |
| 6 C   | -0.400 | -0.416 | -0.374 | 0.026    | 0.016    | 0.021    | 0.01   |
| 7 S   | 0.325  | 0.148  | 0.518  | 0.193    | 0.177    | 0.185    | 0.016  |
| 8 S   | 0.325  | 0.148  | 0.518  | 0.193    | 0.177    | 0.185    | 0.016  |
| 9 S   | 0.325  | 0.148  | 0.518  | 0.193    | 0.177    | 0.185    | 0.016  |
| 10 S  | 0.325  | 0.148  | 0.518  | 0.193    | 0.177    | 0.185    | 0.016  |
| 11 H  | 0.273  | 0.224  | 0.307  | 0.034    | 0.049    | 0.0415   | -0.015 |
| 12 H  | 0.273  | 0.224  | 0.307  | 0.034    | 0.049    | 0.0415   | -0.015 |
| 13 H  | 0.273  | 0.224  | 0.307  | 0.034    | 0.049    | 0.0415   | -0.015 |
| 14 H  | 0.273  | 0.224  | 0.307  | 0.034    | 0.049    | 0.0415   | -0.015 |

where +, - and 0 illustrate nucleophilic, electrophilic, and radical attack, respectively. Table 6 shows the local softness and local electrophilicity indices for selecting atomic locations for the TTF molecule. The greatest values of the entire three local...
electrophilicity reactivity descriptors \((S_k^+, f_k^+, \omega_k^+)\) at 7 S, 8 S, 9 S, 10 S atoms specify that this region is the nucleophile. Also, the maximum value of \((S_k^-, f_k^-, \omega_k^-)\) at 7 S, 8 S, 9 S, 10 S atoms shows that this area is electrophile attack as shown in Table 6. The results show that the S atoms have an electrophile attack and nucleophile attack.

**Table 6:** Local softness and electrophilicity indices of the TTF molecule

| Atoms | \(S_k^+\) | \(S_k^-\) | \(S_k^0\) | \(\omega_k^+\) | \(\omega_k^-\) | \(\omega_k^0\) |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| 1 C   | -0.002    | 0.004     | 0.001     | -0.021    | 0.042     | 0.010     |
| 2 C   | -0.002    | 0.004     | 0.001     | -0.021    | 0.042     | 0.010     |
| 3 C   | 0.007     | 0.004     | 0.005     | 0.068     | 0.042     | 0.055     |
| 4 C   | 0.007     | 0.004     | 0.005     | 0.068     | 0.042     | 0.055     |
| 5 C   | 0.007     | 0.004     | 0.005     | 0.068     | 0.042     | 0.055     |
| 6 C   | 0.007     | 0.004     | 0.005     | 0.068     | 0.042     | 0.055     |
| 7 C   | 0.007     | 0.004     | 0.005     | 0.068     | 0.042     | 0.055     |
| 8 C   | 0.007     | 0.004     | 0.005     | 0.068     | 0.042     | 0.055     |
| 9 C   | 0.007     | 0.004     | 0.005     | 0.068     | 0.042     | 0.055     |
| 10 S  | 0.007     | 0.004     | 0.005     | 0.068     | 0.042     | 0.055     |
| 11 H  | 0.009     | 0.013     | 0.011     | 0.088     | 0.127     | 0.108     |
| 12 H  | 0.009     | 0.013     | 0.011     | 0.088     | 0.127     | 0.108     |
| 13 H  | 0.009     | 0.013     | 0.011     | 0.088     | 0.127     | 0.108     |
| 14 H  | 0.009     | 0.013     | 0.011     | 0.088     | 0.127     | 0.108     |

3.3. Thermodynamic Properties

The thermodynamic properties parameters such as thermal energy (E), entropy (S), and molar heat capacity (Cv) of this compound in the gas phase, solvent phase, and in different temperatures were determined by DFT with the 6-311++G as shown in Table 7 & 8 and Figure 2 & 3. TTF’s thermal energy includes the total kinetic energy of all atoms in this molecule. The study of thermodynamic characteristics is necessary in order to predict the outcome of a chemical reaction[36]. As displayed in Table 7, the thermal energy, entropy, and molar heat capacity values are changed from the gas phase to the solvent medium due to the solvent’s polarity. These parameters are directly proportional to the values of temperature. Also, as temperatures rise, the molecular vibration increases.

![Figure 2: The relation between thermal energy and temperature](image1)

![Figure 3: The relation between heat capacity and entropy with variation temperature](image2)

**Table 7:** The effective of solvents in thermodynamic parameters

|                      | Gas phase | Water | Acetone | THF  | Benzene | CCl4  |
|----------------------|-----------|-------|---------|------|---------|-------|
| E (Thermal) Kcal/Mol | 57.712    | 57.746| 57.722  | 57.720 | 57.708  | 57.682|
| Molar heat capacity (CV) Cal/Mol-Kelvin | 36.540    | 36.549| 36.583  | 36.576 | 36.566  | 36.604|
| Entropy (S) Cal/Mol-Kelvin | 101.146   | 101.112| 100.617 | 100.634| 100.821 | 100.429|
4. Conclusion

In this study, the solvent effect on frontier molecular orbitals, global chemical reactivity descriptors, dipole moment, Mulliken population analysis, and thermodynamic properties was analyzed and interpreted using Gaussian 09 software with the (B3LYP/6-311++G) basis sets. The energy gap calculations demonstrated that electron transport from HOMO to LUMO is significantly easier in the gas phase than in the solvent phase. The hardness, electronegativity, electrophilicity index, nucleofugality, and electrofugality declined as the solvent transitioned from polar to non-polar. Softness and chemical potential, on the other hand, reduced as the solvent changed from non-polar to polar. It also demonstrates that the solvent has no effect on the dipole moments because TTF is a non-polar molecule. Mulliken population analysis for nucleophilic and electrophilic charges distribution successfully estimate the reactive region. Thermodynamic properties such as thermal energy and molar entropy give a useful estimate of Halabja and Garmian university. This work was supported by the university.

We conclude that the TTF compound is an excellent object for theoretical investigations, and thermodynamic properties was analyzed in this study, the solvent effect on frontier molecular orbitals, global chemical reactivity descriptors, dipole moment, Mulliken population analysis, and thermodynamic properties was analyzed and interpreted using Gaussian 09 software with the (B3LYP/6-311++G) basis sets. The energy gap calculations demonstrated that electron transport from HOMO to LUMO is significantly easier in the gas phase than in the solvent phase. The hardness, electronegativity, electrophilicity index, nucleofugality, and electrofugality declined as the solvent transitioned from polar to non-polar. Softness and chemical potential, on the other hand, reduced as the solvent changed from non-polar to polar. It also demonstrates that the solvent has no effect on the dipole moments because TTF is a non-polar molecule. Mulliken population analysis for nucleophilic and electrophilic charges distribution successfully estimate the reactive region. Thermodynamic properties such as thermal energy and molar entropy give a useful estimate of Halabja and Garmian university. This work was supported by the university.

We conclude that the TTF compound is an excellent object for future studies of semiconductor and optoelectronic material.

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