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Density functional theory calculations for electronic, optoelectronic and thermodynamic properties of dibenzothiophene metal complexes

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Abstract

The modelling and geometry optimisation of metal–organic complexes of dibenzothiophene have been done to analyse their electronic, optoelectronic, and thermodynamic properties in the gas phase and in solvent phase (Heptane, Chloroform, Dichloroethane, Ethanol, Acetonitrile, Water). The Density functional theory (DFT) has been used to deduce the properties like polarizability (\(\alpha\)), dipole moment (\(\mu\)), first hyperpolarizability (\(\beta\)), second hyperpolarizability (\(\gamma\)), susceptibility (\(\chi\)), dielectric constant (\(\epsilon\)), refractive index (\(n\)), and thermodynamic properties, using the B3LYP functional and LANL2DZ basis function. The high values of n, \(\chi\), \(\beta\), and \(\alpha\), and the small values of HOMO-LUMO energy gap, and \(\epsilon\) affirm good optoelectronic and electronic applications for the studied molecules.

1. Introduction

Earlier, non-linear optical (NLO) materials were majorly based on inorganic crystals but despite having mechanical and thermal stability, they have limited second order coefficients. From recent times potential researches are dwelling upon organic and metal organic NLO materials [1–5]. For the potential applications in the photonic devices, the search for novel materials having large second order nonlinear optical properties are currently a subject of consideration [6, 7]. Organic molecules being chemically flexible with large and fast nonlinear optical response have already proved to be good materials for nonlinear devices. Because of high NLO susceptibilities, organic and metal–organic complexes are of great research interest [8–10]. To predict non-linearity, researchers have studied various organic and organometallic molecular systems [11–13]. This continued interest in organometallic molecules for large NLO properties has been the motivation for the current work presented.

Of various optoelectronic properties, the electric polarizability is an important property for the investigation of optoelectronic properties of the molecules. It can create an induced dipole moment in a dielectric material in the external electric field’s presence. For low electric field case, the formula \(\mu = \langle \alpha \rangle E\) reflecting linearity of the dipole moment, where \(\mu\) is the dipole moment, \(\langle \alpha \rangle\) is the average polarizability, and E is the electric field, defines the polarizability. The behaviour of dipole moment is not linear for the case of strong fields and is given by the relation \(\mu = \alpha E + \beta E^2 + \gamma E^3\) … where \(\beta\) is the first molecular hyperpolarizability, \(\gamma\) is the second molecular hyperpolarizability. A number of studies have been done to discover these properties for different molecules, like Labidi et al [1–4] studied all-trans hexatriene for the substitution effects on the polarizability and hyperpolarizability, while Atalay et al [15] studied some donor–acceptor oxadiazoles for linear and nonlinear optical properties using Hartree–Fock method; and Zafar et al studied non-linear optical properties of 1, 4-Diamino–9, 10-Anthraquinone [16], and many more [17, 18]. There are studies present on NLO properties for natural pigments also [19].

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The current work aims to predict the electronic, optoelectronic, and thermodynamic properties of the molecules: Cr-complex of thiol-ended dibenzothiophene (Cr-TED) and W-complex of thiol-ended dibenzothiophene (W-TED), using density functional theory (DFT). These molecules are formed by replacing the dangling hydrogen in dibenzothiophene with the sulphur atom. The resultant molecule the thiol-ended dibenzothiophene (TED) has been used to make its metal complexes [20, 21]. The electronic and optoelectronic properties along with thermodynamic properties of these molecules are studied to judge whether the molecules are appropriate for optoelectronic applications or not. The properties are studied in the gas phase as well as solvent phase. Since experimentalist use the molecules in the solvent and solvent could modify the geometry and the optoelectronic properties of the molecule, the need for solvent phase calculations seems to be more fruitful and realistic.

2. Computational methodology

Both the molecules (Cr-TED and W-TED) are optimised using Gaussian 03 software [22] by employing B3LYP functional [23–25] accompanied by LANL2DZ basis set in gas phase and in solvent phase (Heptane (1.9), Chloroform (4.81), Dichloroethane (10.36), Ethanol (24.5), Acetonitrile (37.5), Water (80.1)). The basis set LANL2DZ has been chosen because of the presence of transition metal in the molecules and hence is applied for both the molecules in order to compare the results at same level of theory. Further, calculations to determine mean polarizability ($\alpha$), first molecular hyperpolarizability ($\beta$), average second molecular hyperpolarizability ($\gamma$) and isotropy ($\Delta\alpha$) of the molecular systems are performed using the same functional and basis set.

Due to the inadequacy of gas phase results of the molecules in describing the solution effect, the solvent effect has been studied using Heptane, Chloroform, Dichloroethane, Ethanol, Acetonitrile, and Water as solvent for the molecules. For this process, the self-consistent reaction field (SCRF) theory [26] is used with LANL2DZ basis set.

For the calculation of optoelectronic properties of the molecules, the conversion factors required to convert atomic units to SI units: 1 Debye = $3.336 \times 10^{-30}$ Cm (Coulomb meter), 1 a. u. of $\alpha = 1.64878 \times 10^{-41}$ C$^2$ m$^3$ J$^{-1}$, 1 a. u. of $\beta = 8.6393 \times 10^{-33}$ esu = $3.206361 \times 10^{-53}$ C$^3$ m$^3$ J$^{-2}$, and 1 a.u. of $\gamma = 6.23597 \times 10^{-65}$ C$^4$ m$^4$ J$^{-3}$ [27, 28]. Also, pressure and temperature are set to 1 atm and 298.15 K, respectively for all the thermodynamic property calculations.

3. Results

3.1. Molecular structure and geometrical properties

The ground state geometries of the molecules (TED, Cr-TED, and W-TED) optimised using B3LYP functional employing LANL2DZ basis set for the DFT calculations are shown in the figure 1. The optimised ground state energies are $-13362.88$ eV for TED, $-31129.81$ eV and $-30628.16$ eV for Cr-TED and W-TED, respectively showing relative stabilisation of the molecules.

The selected optimised parameters presented in table 1 for Cr and W complex of Dibenzo thiophene show almost same values for experimental [29] and theoretical case as depicted by percentage difference values.
|                | Cr-TED | W-TED |        | Cr-TED | W-TED |        |
|----------------|--------|--------|--------|--------|--------|--------|
|                | Theoretical | Experimental | % Difference | Theoretical | Experimental | % Difference |
| Cr-S           | 2.6012 | 2.4512 | 3.48   | W-S    | 2.720  | 2.580  | 5.28   |
| Cr-C (2)       | 1.8969 | 1.9090 | 0.63   | W-C (4) | 2.041  | 2.006  | 1.72   |
| Cr-C (4)       | 1.8926 | 1.8984 | 0.30   | W-C (5) | 2.039  | 2.039  | 0.00   |
| Cr-C (6)       | 1.8944 | 1.9218 | 1.43   | W-C (6) | 2.037  | 2.060  | 1.12   |
| Cr-C (5)       | 1.8944 | 1.9030 | 0.45   | W-C (2) | 2.037  | 2.020  | 0.83   |
| Cr-C (3)       | 1.8484 | 1.8550 | 0.35   | W-C (3) | 1.975  | 1.962  | 0.66   |
| S-C (13)       | 1.8459 | 1.7727 | 4.04   | S-C (12)| 1.852  | 1.762  | 4.98   |
| S-C (12)       | 1.8480 | 1.7692 | 4.35   | S-C (13)| 1.851  | 1.764  | 4.81   |
| Angle (degree) | Theoretical | Experimental | Percentage difference | Angle (degree) | Theoretical | Experimental | Percentage difference |
| C(13)-S-Cr     | 112.68 | 109.40 | 3.04   | C(12)-S-W | 109.9  | 110.8  | 0.81   |
| C(12)-S-Cr     | 110.79 | 112.78 | 1.78   | C(13)-S-W | 111.8  | 108.2  | 3.27   |
| C(2)-Cr-S      | 87.82  | 92.81  | 5.52   | C(3)-W-S | 177.2  | 177.1  | 0.05   |
| C(4)-Cr-S      | 87.58  | 88.06  | 0.54   | C(4)-W-C(6)| 178.9  | 178.9  | 0.00   |
| C(6)-Cr-S      | 91.08  | 91.12  | 0.04   | C(2)-W-C(5)| 178.3  | 175.1  | 1.81   |
| C(5)-Cr-S      | 93.05  | 91.78  | 1.37   | C(3)-W-C(4)| 90.2   | 89.3   | 1.00   |
| C(3)-Cr-S      | 176.76 | 177.05 | 0.16   | C(3)-W-C(2)| 89.2   | 89.7   | 0.55   |
| C(12)-S-C(13)  | 89.11  | 91.05  | 2.15   | C(12)-S-W | 109.9  | 110.8  | 0.81   |
| C(4)-Cr-C(2)   | 89.94  | 90.54  | 0.66   | C(3)-W-C(5)| 89.1   | 85.7   | 3.89   |
| C(2)-Cr-C(6)   | 90.07  | 90.77  | 0.77   | C(4)-W-C(2)| 89.8   | 90.9   | 1.21   |
| C(3)-Cr-C(4)   | 89.55  | 89.17  | 0.42   | C(3)-W-C(6)| 90.7   | 90.9   | 0.2    |
| C(3)-Cr-C(5)   | 90.84  | 89.27  | 1.74   | C(2)-W-C(6)| 90.4   | 88.0   | 2.69   |
| C(4)-Cr-C(5)   | 90.60  | 90.72  | 0.13   | C(5)-W-C(6)| 89.4   | 90.4   | 1.11   |
| C(3)-Cr-C(2)   | 89.55  | 86.19  | 3.82   | C(4)-W-S | 87.8   | 88.6   | 0.90   |
| C(5)-Cr-C(2)   | 178.54 | 175.28 | 1.84   | C(2)-W-S | 88.7   | 92.3   | 3.97   |
| C(3)-Cr-C(6)   | 90.84  | 91.67  | 0.90   | C(5)-W-S | 92.8   | 92.4   | 0.43   |
| C(4)-Cr-C(6)   | 179.11 | 178.49 | 0.34   | C(6)-W-S | 91.0   | 91.2   | 0.21   |
| C(5)-Cr-C(6)   | 89.39  | 88.03  | 1.53   | C(12)-S-C(13)| 89.0  | 90.7   | 1.89   |

* Reference [29].
Now to understand molecular chemical stability and the relationship of Nonlinear optical properties with the molecular structure, the HOMOs, LUMOs, and HOMO-LUMO energy gaps have been studied for both the molecules [30]. The HOMO-LUMO energy gap for the optimised molecules in gas phase and solvent (Heptane, Chloroform, Dichloroethane, Ethanol, Acetonitrile, Water) phase are presented in the table 2. It can be observed clearly from table 2 that the $E_g = E_{HOMO} - E_{LUMO}$ values for both the molecules changes on the inclusion of solvation effects. Also, there is an increment in the HOMO-LUMO gap for solvent phase than gas phase for both the metal complexes with increasing dielectric constant of the solvents.

### 3.2. Energies

The first order energy derivative with respect to the applied electric field gives the dipole moment and represents the strength of the polarity of the molecule. The thermodynamic properties like zero-point vibrational energy, electronic energy (zero-point corrected total energy), entropy, enthalpy, and free energy of the molecules: Cr–TED, and W–TED, are presented in table 3. The effects of solvent phase can be seen on the thermodynamic properties, electronic energies are decreasing with increasing dielectric constants of the solvents, hence molecules are getting stabilized in more polar solvents.

### 3.3. Polarizability, hyperpolarizability and second hyperpolarizability

The second order energy derivative with respect to the applied electric field is defined as the polarizability of the molecule. A large variety of physical phenomena are explainable with the help of polarizability. Also, experimental difficulties in obtaining reliable values for polarizability arouses the demand of theoretical results.

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**Table 2.** The HOMO-LUMO energy gap (in eV) of the molecules: Cr–TED, and W–TED.

| Phase         | Cr–TED | W–TED |
|---------------|--------|-------|
| Gas           | 1.5170 | 1.5164|
| Heptane (1.9) | 1.5217 | 1.5249|
| Chloroform (4.81) | 1.5287 | 1.5306|
| Dichloroethane (10.36) | 1.5339 | 1.5254|
| Ethanol (24.5) | 1.5366 | 1.5293|
| Acetonitrile (37.5) | 1.5574 | 1.5303|
| Water (80.1)   | 1.5385 | 1.5459|

**Table 3.** Thermodynamic properties i.e., zero-point vibrational energy ZPVE (kcal/mol), electronic energy $E$ (kcal/mol), entropy $S$ (cal/mol-K), enthalpy $H$ (kcal/mol), and free energy $F$ (kcal/mol) of the molecules: Cr–TED, and W–TED.

| Phase         | ZPVE   | E      | S      | H      | F      |
|---------------|--------|--------|--------|--------|--------|
| Cr–TED        |        |        |        |        |        |
| Gas           | 115.9489 | −717754.2523 | 179.007 | 16.3843 | −36.9860 |
| Heptane (1.9) | 115.7780 | −717758.4591 | 179.517 | 16.4169 | −37.1059 |
| Chloroform (4.81) | 115.6730 | −717762.7205 | 179.149 | 16.4219 | −36.9917 |
| Dichloroethane (10.36) | 115.7592 | −717764.7781 | 177.776 | 16.3793 | −36.6246 |
| Ethanol (24.5) | 115.7852 | −717766.0382 | 178.012 | 16.3755 | −36.6993 |
| Acetonitrile (37.5) | 115.7920 | −717766.3199 | 178.121 | 16.3736 | −36.7332 |
| Water (80.1)   | 115.7451 | −717766.7284 | 178.763 | 16.3912 | −36.9070 |

| Phase         | ZPVE   | E      | S      | H      | F      |
|---------------|--------|--------|--------|--------|--------|
| W–TED         |        |        |        |        |        |
| Gas           | 115.1348 | −706186.4693 | 183.312 | 16.6460 | −38.0083 |
| Heptane (1.9) | 114.9315 | −706190.9904 | 176.319 | 16.1314 | −36.4389 |
| Chloroform (4.81) | 114.8120 | −706195.5298 | 184.503 | 16.7300 | −38.2793 |
| Dichloroethane (10.36) | 114.7418 | −706197.7763 | 186.093 | 16.7520 | −38.7318 |
| Ethanol (24.5) | 114.7549 | −706199.1085 | 186.294 | 16.7432 | −38.8002 |
| Acetonitrile (37.5) | 114.7618 | −706199.4047 | 186.375 | 16.7407 | −38.8272 |
| Water (80.1)   | 114.7209 | −706199.4743 | 177.121 | 16.1835 | −36.6252 |
The B3LYP functional with LANL2DZ basis set are used to obtain the tensor components of polarizability, using these components the average polarizability, the anisotropy, and the averaged second hyperpolarizability for the molecules have been calculated. The six polarizability tensor components for a molecule are given as $\alpha_{x x}$, $\alpha_{y y}$, $\alpha_{z z}$, $\alpha_{x y}$, $\alpha_{x z}$, and $\alpha_{y z}$. These are further used to calculate average polarizability $\langle \alpha \rangle$ and anisotropy $\Delta \alpha$ using the following formulas:

$$\langle \alpha \rangle = \frac{1}{3}(\alpha_{x x} + \alpha_{y y} + \alpha_{z z})$$

$$\Delta \alpha = \frac{1}{2}[(\alpha_{x x} - \alpha_{y y})^2 + (\alpha_{y y} - \alpha_{z z})^2 + (\alpha_{z z} - \alpha_{x x})^2 + 6(\alpha_{x y}^2 + \alpha_{y z}^2 + \alpha_{z x}^2)]^{\frac{1}{2}}$$

and are expressed in the Table 4.

It can be observed that the dipole moments of the metal complexes have changed on the solvent introduction and increase on increasing polarity of solvents. On comparing the gas phase to solvent phase calculations, one can observe an increment in the magnitude of dipole moment for the solvent phase, with a decrement in the energies.

To understand the relation between the nonlinear optical properties and the molecular structure, it is useful to theoretically determine the hyperpolarizability of the molecule. The nonlinear optical activity of the molecule is measured by hyperpolarizability. From table 4, it is found that the polarizability of metal complexes has changed on the inclusion of solvent phase. Also, there is a noticeable change in the values of the polarizability for both the molecules from gas to solvent phase. Also, anisotropy of the molecules has shown an increase in values for the metal complexes on shifting to solvent phase from gas phase.

Table 4 also shows the first molecular hyperpolarizability ($\beta_{mol}$) of the molecules calculated from the 10 components $\beta_{xxx}$, $\beta_{xxy}$, $\beta_{xyy}$, $\beta_{yyx}$, $\beta_{yyz}$, $\beta_{xyz}$, $\beta_{xzx}$, $\beta_{xzy}$, $\beta_{yyz}$, and $\beta_{zzz}$ of the hyperpolarizability. The values are presented in electrostatic units after conversion from the atomic units. The formula used for the calculations are as follows:

$$\beta_{tot} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{\frac{1}{2}}$$

$$\beta_{mol} = \frac{1}{3}(\beta_x^2 + \beta_y^2 + \beta_z^2)^{\frac{1}{2}}$$

Where, $\beta_x$, $\beta_y$, and $\beta_z$ have been calculated using

$$\beta_i = \beta_{ii} + \frac{1}{3}\sum_{j\neq i}(\beta_{ij} + \beta_{ji})$$
As is evident from table 4, the molecular hyperpolarizability for the Cr complex of dibenzothiophene and W complex of dibenzothiophene has shown a decrease in the values with respective solvent inclusion. Also, an inverse relationship of hyperpolarizability with HOMO-LUMO energy gap, \( E_g \) has been observed. This is in conformity with the earlier results reported in the literature. It has also been observed that the values of the hyperpolarizability obtained for the studied molecules (Cr-TED \((0.5030 \times 10^{-30}\) esu), and W-TED \((1.8176 \times 10^{-30}\) esu)) are higher in comparison to that of Urea \((0.1947 \times 10^{-30}\) esu) reported in literature \([31–33]\). Urea is the reference molecule which is used in the study of the nonlinear optical properties of molecular structure. On comparing gas phase to the solvent phase, a clear increase in the molecular hyperpolarizability value for both the molecules can be noted. From the table 4 one can conclude that the polarizability and first hyperpolarizability values for these molecules are sufficiently high to be considered as good option for optoelectronic applications.

The averaged second hyperpolarizability is defined as

\[
\langle \gamma \rangle = \frac{1}{5} \left[ \gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz} + 2(\gamma_{xyyx} + \gamma_{xxyx} + \gamma_{yyzz}) \right]
\]

Where, \( \gamma_{xxxx} \), \( \gamma_{yyyy} \), \( \gamma_{zzzz} \), \( \gamma_{xyyx} \), \( \gamma_{xxyx} \), and \( \gamma_{yyzz} \) are the components of the second hyperpolarizability tensor. The averaged second hyperpolarizability values in gas phase as well as in the solvent phase are presented in table 4 for both the molecules: Cr-TED, and W-TED. From table 4, one can conclude that the averaged second hyperpolarizability values have decreased for the metal complexes from gas phase to solvent phase.

Another important property i.e., Molar Refractivity (MR) related to polarizability by the Lorentz-Lorentz equation is as follows

\[
MR = \frac{(n^2 - 1)(n^2 - 2)MW}{\rho} = 1.333\pi N\alpha
\]

Where, \( n \), \( MW \), \( \rho \), \( N \), and \( \alpha \) are the refractive index, molecular weight, density, Avogadro number, and polarizability of the molecule respectively. On inclusion of solvent, MR shows an increment with increasing dielectric constant of solvents.

### 3.4. Electronic and optoelectronic properties

Depending upon the values of polarizability and dipole moment, the electronic and optoelectronic properties have been calculated. The values of the average electric field \( E \), the polarisation density \( P \), the electric susceptibility \( \chi \), the dielectric constant \( \epsilon_r \), the refractive index \( n \), and the displacement vector magnitude \( D \), of the molecules obtained from B3LYP functional with LANL2DZ basis sets are shown in the table 5. These values of electronic and optoelectronic properties of molecules are obtained from the given equations in the literature \([34]\) as follows

\[
\mu = \langle \alpha \rangle E, \quad P = \frac{\langle \alpha \rangle}{V}, \quad P = \epsilon_0 \chi E, \quad \chi = \epsilon_r - 1, \quad \epsilon = \epsilon_0 \epsilon_r, \quad n = \sqrt{\epsilon}, \quad D = \epsilon E
\]

All symbols have their respective meanings.

### Table 5. Electronic and optoelectronic properties, the average electric field \( E \) (\( \text{Vm}^{-1} \)), the polarization density \( P \), electric susceptibility \( \chi \), refractive index \( n \), the dielectric constant \( \epsilon \), and the magnitude of the displacement vector \( D \) of the molecules: Cr-TED, and W-TED.

| Phase | \( E \times 10^9 \) | \( P \times 10^{-1} \) | \( \chi \) | \( n \) | \( \epsilon \times 10^{-11} \) | \( D \times 10^{-1} \) |
|-------|-----------------|-----------------|-------|------|-----------------|-----------------|
| Cr-TED |                |                |       |      |                |                |
| Gas   | 3.2075          | 1.9179          | 6.7563| 2.7850| 6.8644         | 2.2017         |
| Heptane (1.9) | 2.8188          | 1.7176          | 6.8852| 2.8081| 6.9784         | 1.9671         |
| Chloroform (4.81) | 2.4063          | 2.2989          | 10.7949| 3.4344| 9.5354         | 2.2989         |
| Dichloroethane (10.36) | 2.2046          | 2.6328          | 13.4944| 3.8071| 12.8275        | 2.8279         |
| Ethanol (24.5) | 2.1181          | 2.7140          | 14.4781| 3.9342| 13.6981        | 2.9014         |
| Acetonitrile (37.5) | 2.0577          | 2.6917          | 14.7805| 3.9725| 13.9657        | 2.8738         |
| Water (80.1) | 2.0207          | 2.7535          | 15.3965| 4.0493| 14.5109        | 2.9323         |
| W-TED |                |                |       |      |                |                |
| Gas   | 3.4519          | 1.3974          | 4.5743| 2.3610| 4.9333         | 1.7029         |
| Heptane (1.9) | 3.0216          | 2.0317          | 7.3976| 2.9322| 7.6088         | 2.2991         |
| Chloroform (4.81) | 2.6376          | 2.4566          | 10.5239| 3.9347| 10.1986        | 2.6900         |
| Dichloroethane (10.36) | 2.4213          | 2.7402          | 12.7875| 3.7132| 12.2019        | 2.9545         |
| Ethanol (24.5) | 2.2848          | 2.6349          | 13.0310| 3.7585| 12.4174        | 2.8371         |
| Acetonitrile (37.5) | 2.2544          | 2.2762          | 11.4084| 3.5226| 10.9815        | 2.4757         |
| Water (80.1) | 2.1544          | 2.7575          | 14.4623| 3.9322| 13.6841        | 2.9482         |
The solvent effect on the molecules is such that the values for $P$, $\chi$, $n$, $\epsilon$, and $D$ have changed. Also, a decrease in the values of $E$ is seen for the solvent phase. From table 5 one can see clearly the high values for susceptibility and refractive index, and small values of dielectric constant, polarization density and the displacement vector magnitude. And, the high value of the refractive index of the molecules is due to their high average polarizability. Also, on comparing the results calculated with other metal complexes, the polarizability and hyperpolarizability values are found to be greater for our complexes. Some metal complexes from literature - Mn(II) complex [35] with $\alpha = 43.913 \times 10^{-24}$ esu, - Novel Zn(II) complexes [36] with $\alpha$ ranging from $2.07 \times 10^{-23}$ esu to $4.92 \times 10^{-23}$ esu and $\beta$ ranging from $0.75 \times 10^{-30}$ esu to $2.90 \times 10^{-30}$ esu, - Copper(II) complex [37] with $\alpha = 53.42 \times 10^{-22}$ esu and $\beta = 0.31 \times 10^{-30}$ esu, - Bis(Thiourea) Nickel Bromide (BTNB) [38] with $\alpha = 275.844$ au and $\beta = 60.3088$ au, and some other complexes [39] have lower values of $\alpha$ and $\beta$ than our complexes Cr-TED ($\alpha = 58.02 \times 10^{-24}$ esu and $\beta_{tot} = 1.51 \times 10^{-36}$ esu) and W-TED ($\alpha = 60.50 \times 10^{-24}$ esu and $\beta_{tot} = 5.45 \times 10^{-36}$ esu) and hence are found to be having greater NLO properties, making them more appropriate for electronic and optoelectronic applications.

4. Conclusions

The molecules Cr-TED, and W-TED have been studied for the optoelectronic properties (dipole moment, polarizability, anisotropy, first molecular hyperpolarizability, polarization density, electric susceptibility, refractive index, dielectric constant, the magnitude of the displacement vector of the molecule) and thermodynamic properties (zero-point vibrational energy, electronic energy, entropy, enthalpy, and free energy) using DFT method by employing B3LYP functional and LANL2DZ basis set for gas phase and solvent phase (Heptane, Chloroform, Dichloroethane, Ethanol, Acetonitrile, Water). The $E_g$ of studied molecules shows an inverse relationship with hyperpolarizability and referring to Urea (0.1947 $\times 10^{-30}$ esu) and some other metal complexes, both the molecules have larger values of first molecular hyperpolarizability. Molar Refractivity has been calculated with polarizability. The molecules show second-order optical effects due to their large first hyperpolarizability suggesting potential applications in the field of optoelectronics like charge storage, electroluminescent devices, optoelectronic devices, etc. The molecules come up with high values of refractive index and susceptibility, along with small values of dielectric constant, polarization density and the magnitude of the displacement vector in both gas and solvent phase, leading to optoelectronic properties and applications.

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