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## Quantum Computational Study of the electronic properties of the interactions between 3THF and Some Metallic Linear Molecules Using DFT

<sup>1</sup> Shahad Hayab Talib <sup>2</sup> Abbas Shawai Alwan

<sup>1</sup> Dhi Qar Education Directorate <sup>2</sup> Faculty of Science of Dhi Qar University

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### Abstract:

Some electrical properties were achieved using DFT approach for 3THF-2Cr, 3THF-2Y, 3THF-2Pt and 3THF-2Au at LanL2DZ, B3LYP basis sets. 3THF-2Ni, 3THF-2V, 3THF-2Co and 3THF-2Sc calculations have been investigated throughout 3-21G, B3LYP basis sets (THF point out TetraHydroFuran). Molecular geometry, current surfaces, contour maps, infrared spectroscopy, density of states, HOMO, LUMO electronic states, energy gaps ( $E_g$ ), ionization potentials, electron affinities, hardness, softness, electronegativities, electrophilicities, and polarizabilities were the characteristics that have been studied. The geometrical characteristics of 3THF appear to have been modified by doping with (2Cr, 2Y, 2V, 2Sc, 2Pt, 2Au, 2Ni and 2Co), this happens as a result of the interaction between 3THF and the transition metals. According to the diagrams of surfaces one can visualize that the charges distribute around atoms in 3THF-Ni dramatically tremendously in different way as compared with 3THF-2Y and 3THF-2V. The contour maps clarify how the atoms in THF exchange the electrons with metallic molecules, also this property i.e. density contours describe charge transfer procedure. Infrared spectra figures show apparently the new bonds that result because of the interaction between 3THF atoms and acceptor atoms (metallic transition). 3THF-Pt has around only one peak although the interaction between 3THF atoms and metallic atoms this is take place because of shielding procedure making the interaction with some atoms more than the others. Density of states (DOS) sketches show that 3THF-2Sc has the highest value of DOS around 4.4 at (-10 eV) as compared with 3THF and other coordination complexes, one can say new electronic levels demonstrate the electrons can occupy. Addition of transition metals to 3THF reduce the energy gap values, 3THF-2Y has about (2.1147 eV) energy gap, but 3THF has the value (6.4248 eV), this is very beneficial in the electronic manufacture. Also one can see influence of addition of transition metals to 3THF by spotting the tables of ionization potential, electron affinity, hardness, softness, electrophilicity, electronegativity and average polarizability, as example, hardness value decrease from (3.2124 eV) for 3THF to (1.0573 eV) for 3THF-Au, another example electrophilicity value increased in (3THF-2V) to become (4.0779), when it was around (1.2342 eV) in 3THF.

**Keywords:** DFT, B3LYP, HOMO, LUMO, Energy gap, HSAB, Polarizability.

### 1. Introduction

#### 1.1. Quantum Computational Methods

Density Functional Theory (DFT) is a computational method that employs quantum mechanics and quantum chemistry to investigate the electronic structure (basically the ground state level) of many electron systems, including nanoclusters, using sophisticated algorithms in the Gaussian 09 software [1][2][3]. Instead of functions, functionals are used in DFT. Functionals are functions that are functions of other functions. Instead of dealing with the wave function, DFT deals with electron density  $\rho(r)$ . [4][5][6]. DFT is now used in solid state physics and solid state chemistry calculations. DFT has progressed over time. Day after day, scientists solve problems in order to achieve the highest accuracy in physics and biochemistry calculations. For example, until the 1990s, DFT was not considered precise enough for

quantum chemistry calculations because the approximations used in the theory at the time did not have the best model for description exchange and correlation interactions [7][8][9]. Nowadays, the results of DFT accord satisfactorily with the values obtained from practical data. In DFT computations, basis sets are used. Basis sets are functions that characterize the orbitals according to molecular orbital theory, such as LanL2DZ, LanLMB, and the hybrid functional (B3LYP). In 1993, Alex Becke proposed the hybridization approach for describing correlation exchange energies. DFT computations are carried out as part of the geometry optimization phase; this procedure begins with primary geometry and then moves on to new geometry requirements in a 128-cycle cycle using complex algorithms in Gaussian 09 [10][12]. This is done until the minimal energy geometry is found, at which point the force on each atom is calculated by computing the gradient, which is the first derivative of the energy with respect to the atomic locations. To reach the most stable state, the force acting on the atoms must eventually equal to zero [13] [14].

### 1.2. Coordination compounds:

An atom, a small group of atoms, or a molecule that is connected to a metal atom is referred to as a ligand. A coordination complex is formed when an atom, an ion, or a molecule interacts with a transition metal. The ligand, which is made up of atoms, ions, and molecules, will act as a donor in the coordination compound, while the metal will act as an acceptor [15-17]. The transition metal possesses d orbitals, and the electron pairs in the ligand can occupy the empty d orbital in the transition metal, forming a coordinating connection between the ligand and the metal. Ligands give electron pair which has the capability of linkage by sigma ( $\sigma$ ) bond with the metal. Also ligands use ( $\pi$ ) electrons in the connection such as ( $C_2H_2$ ) and ( $C_6H_6$ ). Some ligands can occupy two, three, or even four central atoms in the same compound coordination sites [18-20]. When the complexes form, the acceptor metal is referred to as Lewis acid, while the donor material (electron pair) is referred to as Lewis base. Both cluster and nanocluster of metallic are substances that have metal-metal bonds. Traditional covalence theories do not apply to coordination molecules. According to Warner's (1893) hypothesis, every metal has two types of covalence: elementary, or oxidation case, and secondary, or coordination number. Each metal tries to saturate both the oxidation case and the coordination number of its covalents [21-23]. Complexes are more important in many fields of knowledge, including as medicine, where haemoglobin and the B12 vitamin in the human body are examples of complexes. B12 vitamin is essential for the brain and nervous system in the human body, as haemoglobin transports oxygen from the lungs to the tissues [24-26].

### 1.3. TetraHydroFuran (THF):

Tetrahydrofuran (THF) is a colourless, transparent liquid with an ether-like odor. PTMEG, medicinal solvents, adhesives, PVC cement, and magnetic tape are some of the most common applications for THF. THF has a molecular weight of 72.11 g/mol, an empirical formula of  $C_4H_8O$ , and a freezing point of  $-108^\circ C$  ( $-162.4^\circ F$ ). It should only be stored in a firmly sealed container away from heat sparks and open flames or strong oxidizing agents. Tetrahydrofuran should be handled as follows: Because it is a carcinogen and flammable, this chemical is on the special health hazard substance list. carcinogenic - proceed with caution. Tetrahydrofuran has the potential to irritate the lungs. Bronchitis with cough and phlegm may result from repeated exposure, and/or shortness of breath medical Tetrahydrofuran have five membered ring, Tetrahydrofuran can donate an electron pair to a transition metal in order for it to act as a ligand [27-30].

## 2. Calculations and Discussion:

### 2.1. Molecular Geometry:

The arrangement of atoms in a system can be used to indicate the molecular structure of that system. The configuration of atom locations in the molecule is a critical aspect in achieving the best structure. Throughout the final geometry of the molecule, values of bond angles, bond lengths, and dihedral angles have been chosen with the geometrical optimization procedure taking into account quantum physics concepts. Understanding the molecular structure provides crucial information for determining critical physical quantities such as polarizability and magnetic properties [31] [32]. The methodologies and basis sets that had been used to optimize the structure of 3THF-2Cr, 3THF-2Y, 3THF-2Pt and 3THF-2Au at

LanL2DZ, B3LYP basis sets. But for the structures 3THF-2Ni, 3THF-2V, 3THF-2Co and 3THF-2Sc are 3-21G, B3LYP basis sets.



Figure (1)  
Molecular geometry of 3THF



3THF-2Cr



3THF-2Ni



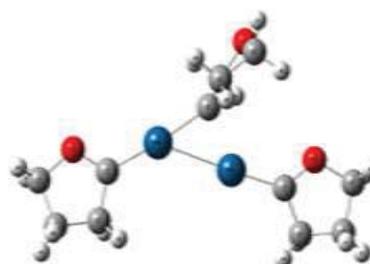
3THF-2Y



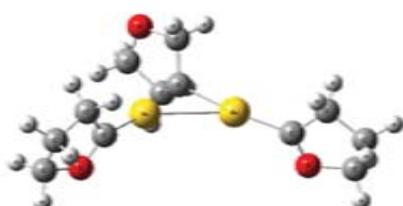
3THF-2V



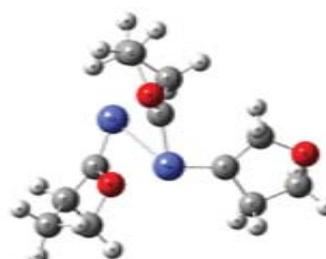
3THF-2Sc



3THF-2Pt



3THF-2Au



3THF-2Co

Figure (2) :Molecular geometry of 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co

One can visualize in figures (1) and (2) the geometries of 3THF and the coordination compounds 3THF-M (M = 2Cr, 2Ni, 2Y, 2V, 2Sc, 2Pt, 2Au and 2Co) where (Cr= chromium ,Ni= nickel,Y= Yttrium,V= Vanadium,Sc= Scandium,Pt= Platinum,Au=gold. One visualize apparently that one of Oxygen atoms in the coordination complex 3THF-2V take close location of the transition metal, as compared with 3THF-2Pt Oxygen atom take relatively far location of 3THF. Geometry optimum procedure make the transition metallic atoms closed one to other in 3THF-2Cr and 3THF-2Y, i.e. Cr-Cr bond and Y-Y bond are small as compared with Au-Au bond and Sc-Sc bond in 3THF-2Au and 3THF-2Sc respectively. Many parameters may impact the geometrical structure, symmetry, hybridization procedure, and nature of bonding. Geometry optimization process requires the system reach to equilibrium state. In the interactions under the study THF molecules behave as a donors, therefore they are ligands, but the transition atoms play the acceptor role.

## 2.2. Current Surfaces:

Surface is a two-dimensional figure with length, width but no thickness or height. The electrostatic potential can be expressed in terms of the surface using Gaussian 09. The electrical states HOMO and LUMO are clearly produced by surfaces. After completing the geometrical optimization technique, high occupied molecular orbitals and low empty molecular orbitals can be found by selecting MOs in Gaussian 09, which displays a surface image using the Gauss view program. When Gaussian 09 algorithms discover a stationary point at the potential surface, the geometrical optimization operation comes to an end [33] [34]. The optimization approaches and basis sets that had been employed the current surfaces of 3THF, 3THF-2Cr, 3THF-2Y, 3THF-2Pt, 3THF-2Au were DFT method at LanL2DZ, B3LYP basis sets. 3THF -2Ni, 3THF -2V, 3THF -2Co and 3THF-2Sc current surfaces had been achieved at DFT with 3-21G, B3LYP basis sets.

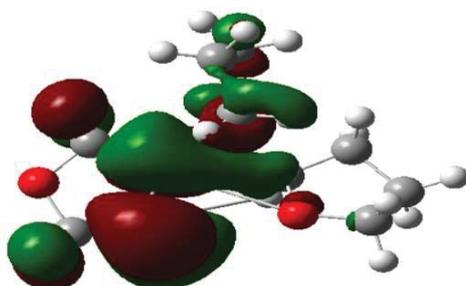
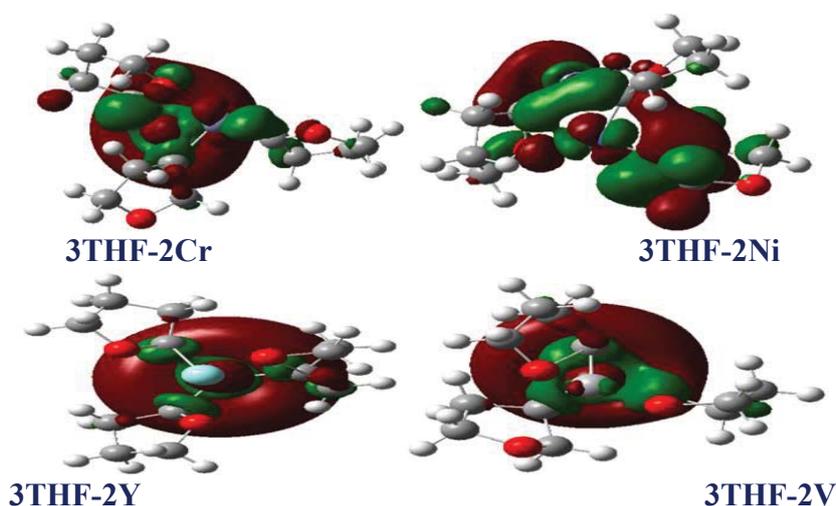
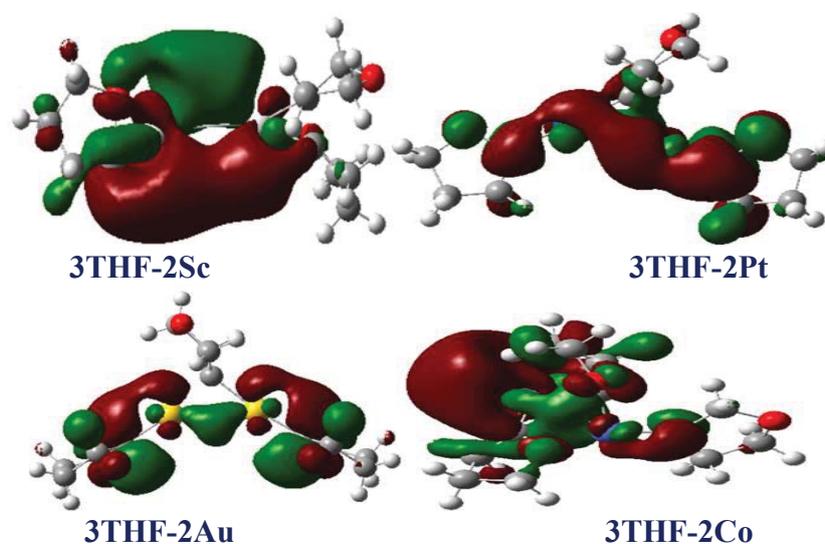


Figure (3)  
Current surface for 3THF



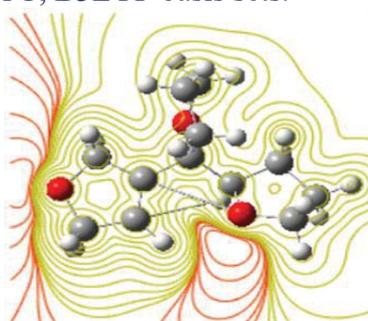


**Figure (4):** Electrostatic potential of 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co

One can visualize in the figures (3) and (4) that decoration charge density in 3THF-2Y and 3THF-2V approximately similar, one can give an interpretation to this behavior, the interpretation is diatomic Yttrium and diatomic Vanadium have convergent behavior when they are interacting with 3THF. By spotting the diagram of coordination complex 3THF-2Au can observe symmetry around the two gold atoms, one can say Au atoms cause this symmetry. The geometrical figure of all coordination compounds 3THF-M, (M = 2Cr, 2Ni, 2Y, 2V, 2Sc, 2Pt, 2Au and 2Co) differs from the geometrical figure of the surface of 3THF, this variety in geometrical figures give a clear picture of the influence of transition metals on the electrostatic potential in the coordination complexes. The potential surfaces emerge because the interactions between the atomic orbitals, potential surfaces describe the molecular orbits which stand for linear synthesis of the atomic orbits. The new orbitals that generate in the coordination compound as a result to the interplay between ligands and transition atoms may be of the type  $\sigma$ ,  $\sigma^*$ ,  $\pi$ ,  $\pi^*$ ,  $\delta$  or  $\delta^*$ . One of the interpretations of the new colors (green and red) in the figures are the green color point out the positive potential, but the red color refers to the negative potential.

### 2.3. Contour Maps:

The density of electronic charges is represented by contours. Another way to describe contour maps is to implement the terms brillion zones, or electrostatic potential and Fermi surface. Density contours describes interaction mechanisms by finding active locations in the molecular structure. The contour principle can also be very beneficial to interpret charge exchange, charge transferring, and electron density distribution in space [35] [36]. The density contour maps had been tweaked for the best results of 3THF-2Cr, 3THF-2Y, 3THF-2Pt and 3THF-2Au at LanL2DZ, B3LYP basis sets. But for the structures 3THF-2Ni, 3THF-2V, 3THF-2Co and 3THF-2Sc are 3-21G, B3LYP basis sets.



**Figure (5)**  
**Electron density distribution around 3THF**

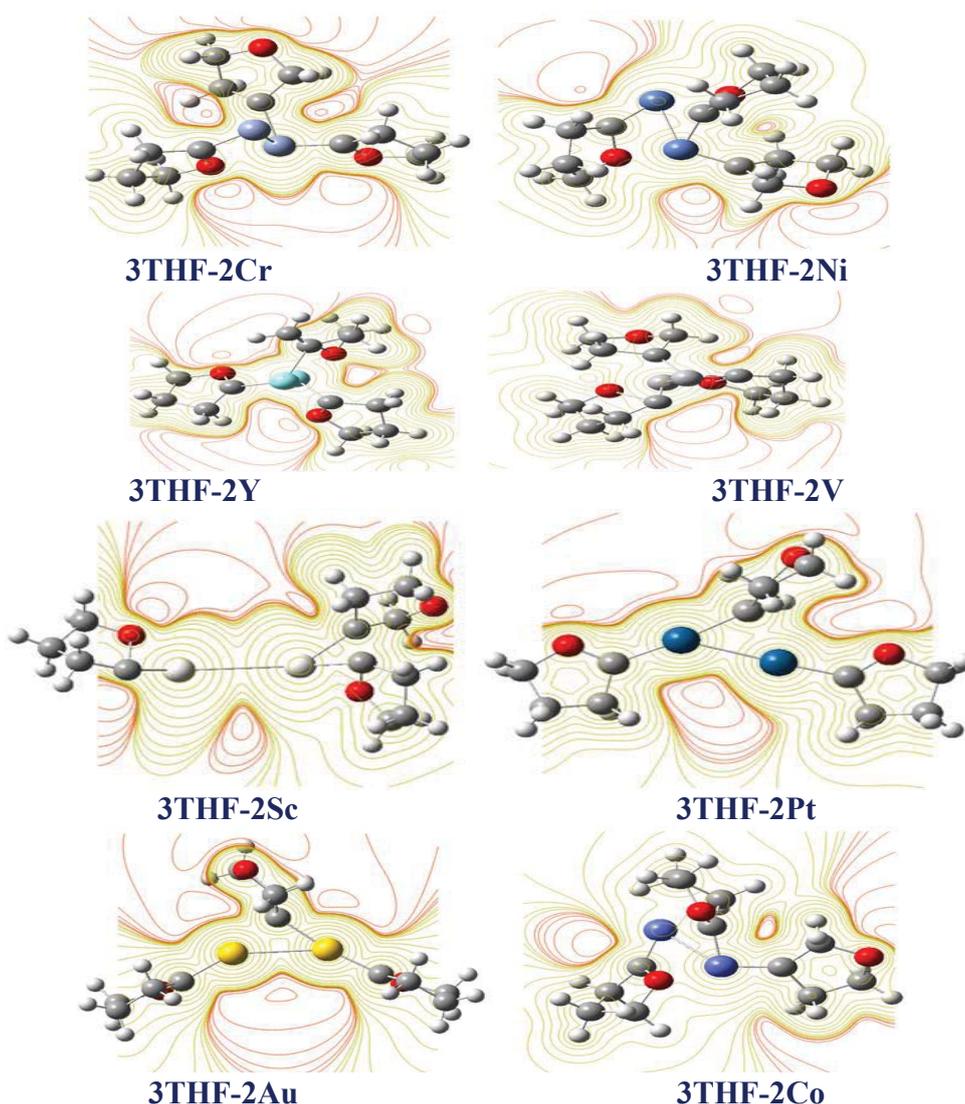


Figure (6) : Electron density distribution around 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co

In the figures (5) and (6) someone can give a description to the spatial distribution of the transition atoms with THF surfaces (contour maps explain this). Contour maps yield the interaction behavior and the probability of happening the overlap, new orbital will originate, the electrons will be able to occupy these orbitals to represent quantum states. Also density contours distortion explain probability of obtaining resonance charge transfer, i.e. electrons will transfer from valence band to the conduction band, this takes place pretty much at three layers of the solid state. Addition of transition metal to 3THF make the decoration of the coordination compounds dissimilar the decoration of 3THF, one can summarize that the spatial distribution of electrons around atoms will become vividly distinction in the interaction ligand-metal. Hence one can say addition of transition metal diatomic molecules to 3THF surfaces lead to distortion in contour maps quit difference as compared with charge distribution in 3THF.

#### 2.4. Infrared Spectra:

The interaction of infrared radiation with materials can be described by infrared spectra plots. Infrared spectra are created by recognizing the ability to absorb infrared light and then transmit it through the vertical centerpiece. It can be shown that the infrared spectra provide information about the symmetric or asymmetric vibrational modes. The symmetric modes are the result of oscillation between atoms of the same species, whereas the asymmetric modes are the consequence of vibration between atoms of different species. Each vibrating mode has its own energy, and each peak of IR spectra can indicate whether the

vibration is elastic or inelastic. IR spectroscopy is used in chemical labs to distinguish between substances. When a material is exposed to IR spectrum, the electric field of the infrared wave interferes with the electric field of the dipole moment [37] [38]. IR spectroscopy theoretically has been investigated for 3THF-2Cr, 3THF-2Y, 3THF-2Pt and 3THF-2Au at LanL2DZ, B3LYP basis sets. But for the structures 3THF-2Ni, 3THF-2V, 3THF-2Co and 3THF-2Sc are 3-21G, B3LYP basis sets.

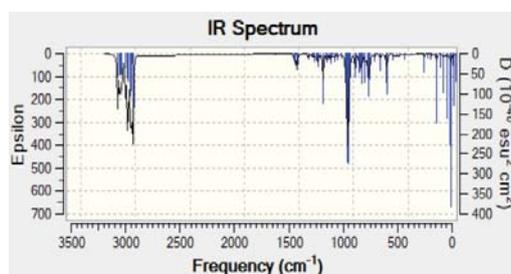


Figure (7) Infrared spectra for 3THF

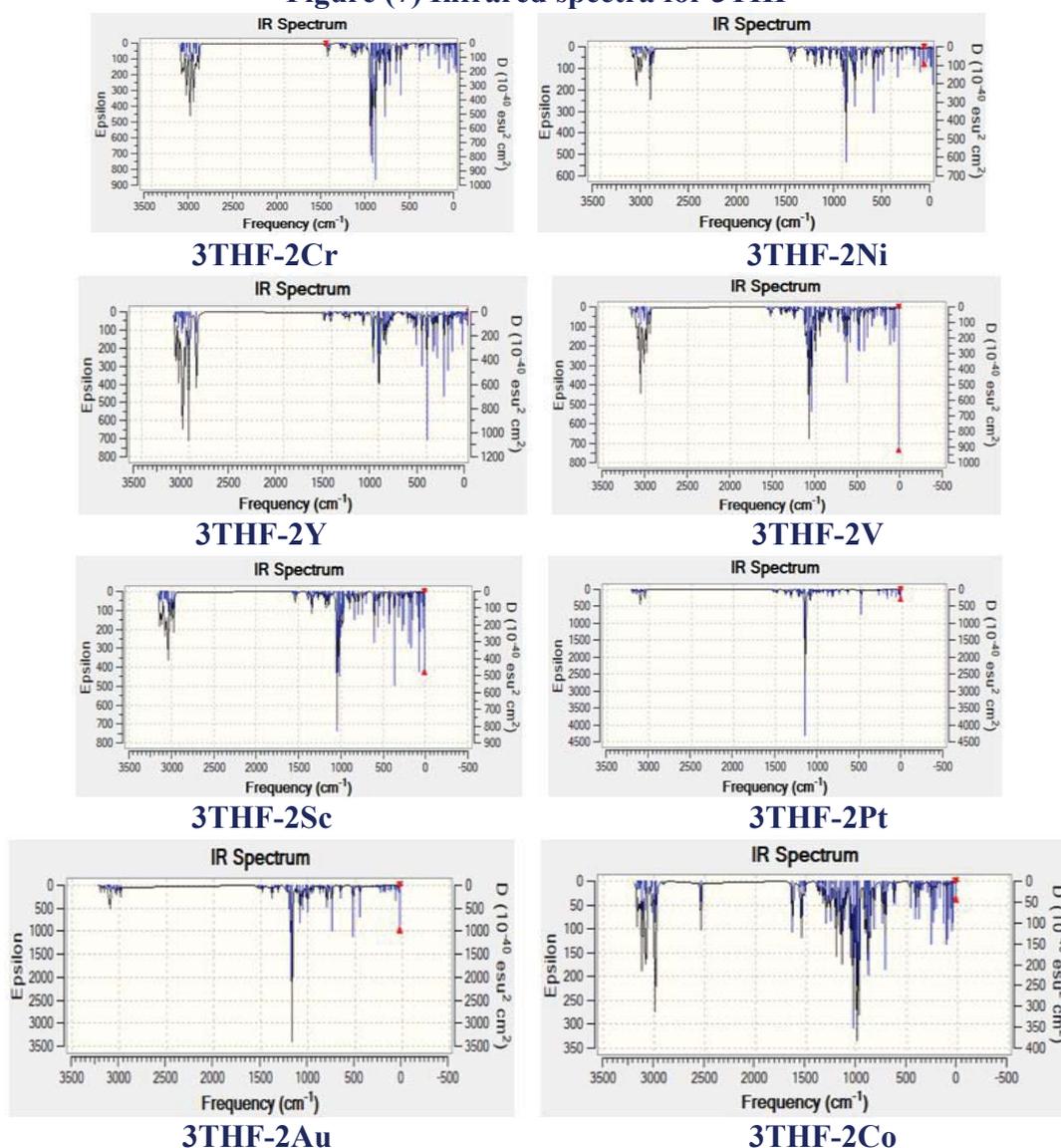


Figure (8): Infrared Spectra for 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co

Figures (7) and (8) depict diagnostic the samples under study theoretically by using sophisticated codes in Gaussian09. In the figures one can scan to make a comparison between 3THF and ligand-metal

nanoclusters, one can inspect new peaks appear in some coordination compounds which are not found in 3THF, otherwise peaks in 3THF disappear when 2Au adds to 3THF, the new peaks sign new bonds formation between 3THF atoms and the transition metal atoms, but the disappearance of the apex can be attributed to shielding procedure obtaining as a result to overlap between gold atoms and 3THF atoms, one can impute this phenomena to tendency of some 3THF atoms to interact with Au atoms more than other atoms in 3THF. One can observe some of new peaks in the coordination compounds have relatively low intensity (at around 100 km/mole). Transition metals have empty d orbitals, therefore coordinating bond will originate between the ligand and transition metal, this lead to attract the electrons from 3THF to occupy laces in d orbital in the transition metals.

### 2.5. Density of states (DOS):

The density of state characteristic can be used to determine the capability of electrons to occupy energetic levels in orbitals, electrons subsistence in energetic levels typify quantum states. In solid state physics, density of states verily can be exist for electrons, phonons, and photons. Quantum statistical physics concepts must be taken into account when electrons occupy the orbits, i.e., electrons ought to subject to Fermi-Dirac statistics, phonons and photons must obey the Bose-Einstein statistic, and electrons must certainly obey Pauli's exclusion principle because they are Fermions. Many parameters, such as topological features, symmetry and geometrical parameters have a significant impact on the density of states [39] [40]. Density of states (DOS) diagrams have been achieved for 3THF-2Cr, 3THF-2Y, 3THF-2Pt and 3THF-2Au at LanL2DZ, B3LYP basis sets. But for the structures 3THF-2Ni, 3THF-2V, 3THF-2Co and 3THF-2Sc are 3-21G, B3LYP basis sets

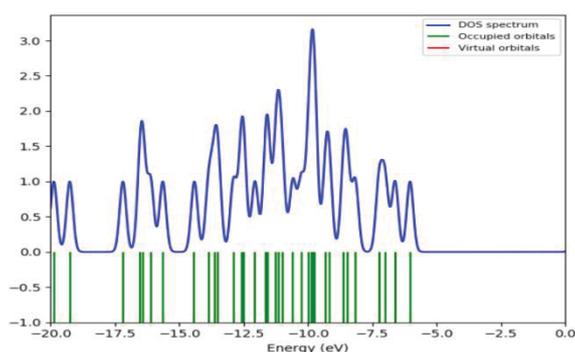
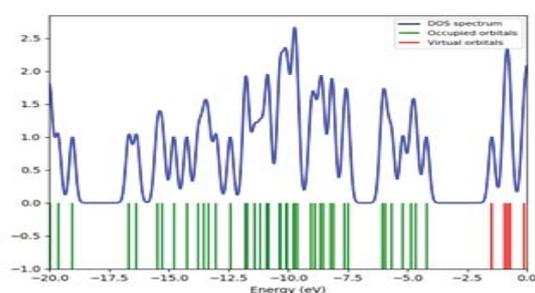
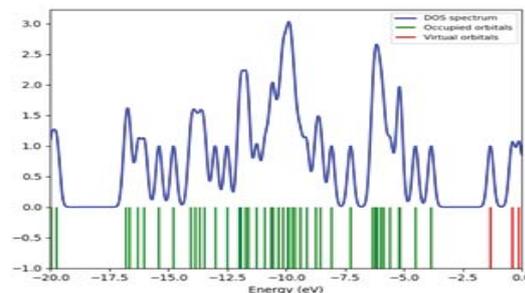


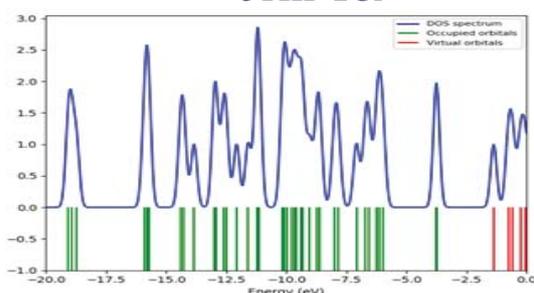
Figure (9) Density for states of 3THF



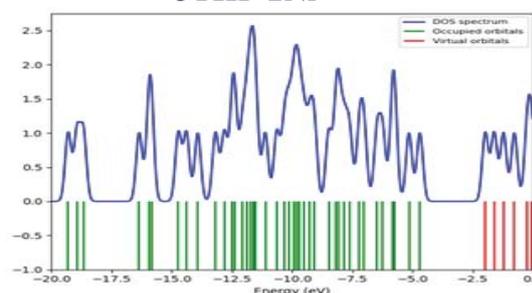
3THF-2Cr



3THF-2Ni



3THF-2Y



3THF-2V

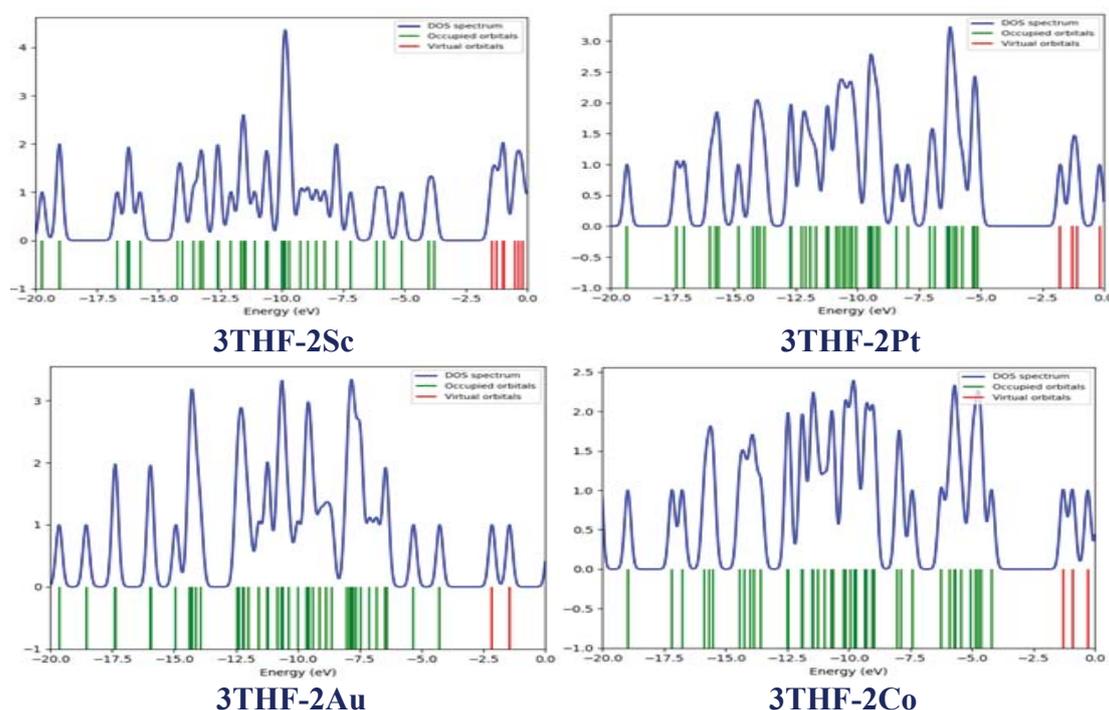


Figure (10): Density of states for 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co

Figures of density of states (9) and (10) describe how the electrons exist in the energy levels, i.e. it clarify band bends, the green and red colors refers to the valence and conduction band. Local density of states obtains as a result to distortion in the system, it causes local vibrations around the equilibrium position. If the density of state zero, the local potential is not zero, therefore the local density of state is not equal to zero. Density of state influence dramatically with the electron density. It is very vivid that the highest apex in 3THF at approximately the density of state 3.2 under (-10 eV), but the highest apex in the coordination compound 3THF-2Sc demonstrate at approximately the density of state 4.4 under (-10 eV), the increase in the value of density of state may denotes to new energetic levels appear in the nanocluster 3THF-2Sc, these levels can be occupied by electrons. Many parameters impact extensively the density of states, molecular geometry, topological properties, hybridization, geometrical parameters and symmetry.

## 2.6. Electronic states and energy gap ( $E_g$ ):

Energy gap is a physical quantity point out the energy that the electron needs to transfer from valence band into the conduction band. The energy that the electron need to immigrate from the valence band to the conduction band of solid material ought to equal or bigger than band gap of the same solid substance. The energy difference between the valence band and the conduction band can be used to compute energy gap values; another definition of energy gap is the energy difference between a high occupied orbit and a low unoccupied orbit. Because of the interference between the valence band and the conduction band, the energy gap for metals is zero. The energy gap in insulators is really large. Temperature and impurities have an impact on the energy gap of semiconductors. The energy gap property can be utilized to distinguish between conductors, semiconductors, and insulators. The energy gap is mathematically expressed as [41] [42]

$$E_g = E_V - E_C \quad \dots \quad (1)$$

Another math formula is also express the energy gap

$$E_g = E_{LUMO} - E_{HOMO} \quad \dots \quad (2)$$

**Table (1) HOMO, LUMO energies and energy gaps (E<sub>g</sub>) of 3THF, 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co**

System	E <sub>LUMO</sub> (eV)	E <sub>HOMO</sub> (eV)	E <sub>g</sub> (eV)
3THF	0.3964497	-6.0283755	6.4248252
3THF-2Cr	-1.4674353	-4.2091149	2.7416796
3THF-2Ni	-1.3264875	-3.8434125	2.516925
3THF -2Y	-1.3673025	-3.72777	2.3604675
3THF-2V	-1.970004	-4.6858341	2.7158301
3THF-2Sc	-1.4538303	-3.8001486	2.3463183
3THF-2Pt	-1.7670174	-5.1048681	3.3378507
3THF-2Au	-2.1465969	-4.2613581	2.1147612
3THF-2Co	-1.2919308	-4.1987751	2.9068443

In Table (1) the LUMO and HOMO values can be seen and the energy gap (for example) of the HOMO orbitals results from the overlap between the atomic orbitals. In metals, the electron pairs of carbon in the p orbital or oxygen in the p orbital can occupy empty d orbitals, acting as donors, transferring electron pairs to metal atoms to form molecular bonding orbitals, either directly or through a linear synthesis of p atomic orbitals in carbon and d orbital in metals. From the table, it can be seen that the lowest energy gap value is for 3THF-Au with about (2.1147 eV), this value is very crucially in the electronic application because it is on the range of a semiconductor band gaps. The impurities (2Cr, 2Ni, 2Y, 2V, 2Sc, 2Pt, 2Au and 2Co) cause dramatic change in the values of band gaps it change from the range of insulators to the range of semiconductors. The electrons that rotate in the outer shells possess more scalar of energy, it link to the nucleus with less attraction force, therefore, it determine the electronic properties to the material. Hence here the decrease in energy gap values means enhancement electronic properties of materials.

### 2.7. Ionization Potential (I.P) and Electron Affinity (E.A):

Enough energy should be available to achieve electron ionization. Ionization potential and electron affinity are two parameters that characterize the binding force of electrons with atoms. Ionization energy is the lowest energy required for an electron to become free from the surface of a molecule or an atom. Because there is only one electron in the outer shell of a hydrogen atom, it has one ionization energy; however, an atom with more than one electron in the outer shell will have ionization energy for each electron. Electron affinity denotes an atom's or molecule's ability to take an electron, in other words, electron affinity denotes a molecule's or atom's trend to acquire an electron. Koopman provided a mathematical equation for calculating ionization potentials and electron affinities according to DFT [43] [44]

$$I.P = -E_{HOMO} \quad \dots (3)$$

$$E.A = -E_{LUMO} \quad \dots (4)$$

**Table (2) demonstrate the ionization potential and electron affinities of 3THF, 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co**

System	I.P(eV)	E.A(eV)
3THF	6.0283755	-0.3964497
3THF-2Cr	4.2091149	1.2919308
3THF-2Ni	3.8434125	1.3264875
3THF -2Y	3.72777	1.3673025
3THF-2V	4.6858341	1.970004
3THF-2Sc	3.8001486	1.4538303
3THF-2Pt	5.1048681	1.7670174
3THF-2Au	4.2613581	2.1465969
3THF-2Co	4.1987751	1.2919308

In Table (2), it is easy to notice that among the coordination complexes under investigation, 3THF-2Y has the lowest ionization potential (around 3.7277 eV). It can be declared that 3THF-2Y is the coordination compound that requires the least amount of energy to be break free the surface of the complex, i.e. it needs the lowest energy to become a cation. The highest value of electron affinity is for 3THF-2Au coordination compound; it is approximately (2.14659eV). One can visualize in the table of ionization potentials and electron affinities adding impurities (2Cr, 2Ni, 2Y, 2V, 2Sc, 2Pt, 2Au and 2Co) to 3THF make the values of ionization potential low, this can deem an improvement in the electronic properties of complexes compounds as compared with 3THF. Ionization potential signs strength of bonds. Ionization potential and electron affinity is very necessary in the calculations of chemical potential and chemical hardness. One can see when censor the values of ionization potentials, it influences with kind of impurity. Ionization energy also describe linkage strength the electron with the atom, this value signs difficulty or simplification of electron with surface. The strength of the acceptor coordination complex is measured by the electron affinity characteristics (E.A) which typify the energy released through addition one electron to LUMO.

### 2.8. Hardness Softness Acid Base (HSAB Principle):

The HSAB concept is based on the Lewis acid base principle, which is primarily used to describe the interaction mechanism. Ralph Pearson first developed this notion (HSAB) in the 1960s. The resistance of a cloud of atoms to polarization and deformation is expressed by its hardness. These two features are particularly advantageous in the fields of chemistry and physics . Acids are classed as hard or soft according to HSAB, too bases are classified similarly. In terms of mathematics according to DFT ideology, The following formulas can be used to calculate hardness and softness, respectively [45] [46].

$$\eta = \frac{I.P-E.A}{2} \quad \dots \quad (5)$$

$$\sigma = \frac{1}{2\eta} \quad \dots \quad (6)$$

**Table (3) demonstrate the Hardness Softness Acid Base of 3THF, 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co**

System	Hardness(eV)	Softness(eV)
3THF	3.2124126	0.155646258
3THF-2Cr	1.3708398	0.364739921
3THF-2Ni	1.2584625	0.39731021
3THF -2Y	1.18023375	0.423644892
3THF-2V	1.35791505	0.368211546
3THF-2Sc	1.17315915	0.426199634
3THF-2Pt	1.66892535	0.299593987
3THF-2Au	1.0573806	0.472866629
3THF-2Co	1.45342215	0.344015674

Table (3) shows that 3THF-2Pt has the highest hardness nanocluster (about 1.6689 eV) among all coordinating compounds studied, but the lowest softness value (around 0.2995 eV) among all coordination complexes, which is due to the fact that hardness and softness are inversely related. 3THF-2Au has the lowest hardness value of about (1.0573 eV), so it has the highest value of softness, also this due to the inverse relationship between hardness and softness. Charge transfer and charge exchange between the transition metals and 3THF may be described described by these two properties. Hardness is an impact factor for description the stability of the system. Also Hardness is very important factor to determine the activity of substances. The impurities cause decreasing in the values of hardness, otherwise, the impurities cause increasing in the values of softness, one can censor this when make a simplifies rapprochement between values of hardness and softness for 3THF and the coordination complexes. Also here sort of impurity effect on the values of hardness and softness.

### 2.9. Electronegativity and Electrophilicity:

Electronegativity is a property that measures an atom's ability to attract a pair of electrons. Linus Pauling proposed the concept of electronegativity in 1932. Other characteristics such as bond energies, ionization energies, electron affinities, HOMO energy, and LUMO energy are impact parameters on the values of those two quantities. Electrophilicity idea, also known as electron lover, participates in interactions by accepting electron pairs in order to attach to nucleophile. As a result, it may be used to look for electron pairs accessible for bonding on atoms or molecules. According to DFT, the following arithmetic equations reflect the mathematical formulas used to compute electronegativity and electrophilicity [47] [48]

$$\chi = \frac{I.P + E.A}{2} \quad \dots (7)$$

$$\omega = \frac{\chi^2}{2\eta} \quad \dots (8)$$

**Table (4) demonstrates the values of electronegativity and electrophilicity of 3THF, 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co**

System	$\chi$ (eV)	$\omega$ (eV)
3THF	2.8159629	1.23421989
3THF-2Cr	2.8382751	2.938273875
3THF-2Ni	2.58495	2.654813514
3THF -2Y	2.54753625	2.749430333
3THF-2V	3.32791905	4.077959517
3THF-2Sc	2.62698945	2.941235028
3THF-2Pt	3.43594275	3.536917508
3THF-2Au	3.2039775	4.854199056
3THF-2Co	2.74535295	2.592833342

Table (4) summarizes manipulation of impurities on the values of electronegativities and electrophilicities. One can visualize that the values of electrophilicity for all coordination complexes nanoclusters (3THF-Metal) larger than the value of electrophilicity of 3THF, one can say addition the impurities (2Cr, 2Ni, 2Y, 2V, 2Sc, 2Pt, 2Au and 2Co) to 3THF lead to increase the values of electrophilicity. Electrophilicity property utilize effectively in the analysis of chemical substances, and it depend on second order expansion of energy with respect to charge transfer (at second geometry), it describe stability of the system. Electrophilicity rely dramatically on the chemical potential and chemical hardness. Also one can put it type of impurity is an effective factor in determining the values of electrophilicity. Electronegativity is an important quantity to determine the type of the bond. Also electronegativity effect on determination direction of polar of chemical bonds. One can observe in the table that the values of electronegativities impact randomly after adding the impurities to 3THF, to explain this, when 2Ni adds to 3THF the value of electronegativity decreased, otherwise after addition of 2Pt to 3THF the value of electronegativity increase (these values of electronegativities are around 2.8159 eV for 3THF, and around 2.5849 eV for 3THF-Ni, but for 3THF-2Pt around 3.4359 eV), this happen because of many parameters like molecular geometry, topological properties and symmetry.

### 2.10. Polarizability:

Polarizability notion denotes to the system's polarization capability as well as the linear response to electron density in the presence of an electric field. It provides information on a substance's internal structure. It is classified as a second-order variation. In the Gaussian 09 results, the values of polarizabilities ( $\alpha_{xx}$ ,  $\alpha_{yy}$ ,  $\alpha_{zz}$ ) can be found in the consequences of Gaussian09. One can utilize the equation below to calculate the average polarazibility [49] [50]

$$\alpha = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad \dots (9)$$

**Table (5) the magnitudes of polarizabilities of 3THF, 3THF-2Cr, 3THF-2Ni, 3THF-2Y, 3THF-2V, 3THF-2Sc, 3THF-2Pt, 3THF-2Au and 3THF-2Co**

System	$\alpha_{xx}$	$\alpha_{yy}$	$\alpha_{zz}$	$\langle \alpha \rangle$
3THF-2Cr	133.117	142.633	99.986	125.2453333
3THF-2Ni	294.57	197.017	161.493	217.6933333
3THF -2Y	245.516	224.51	150.484	206.8366667
3THF-2V	366.04	357.129	408.882	377.3503333
3THF-2Sc	228.375	186.687	163.343	192.8016667
3THF-2Pt	371.568	242.086	218.306	277.32
3THF-2Au	361.798	213.183	147.876	240.9523333
3THF-2Co	438.92	219.07	158.912	272.3006667
3THF-2Cr	245.724	217.174	151.652	204.85

Table (5) summarize polarizabilities of 3THF and the coordination complexes. The (ligand-metal) 3THF-2V has the highest polarizability value, which is around (377.3503 a.u), this indicates that the 3THF -2Y coordination complex has the most vitality and activity. Polarizability provides information around dipole moments and internal structure. Polarizability is very important idea to obtain an approximated values of the effective charges over the molecule. Polarizability represent derivative of second order with respect to Cartesian components. The highest values of polarizabilities is very beneficial in the nonlinear optics branch of knowledge applications. Dipole moment (permanent or induced) is an impact factor relate to the polarizability, so symmetry and geometrical paramters are important coefficients manipulate on the polarizability. Kind of impurity also manipulates on the values of polarizabilities.

### 2.11. Conclusions:

When linear transition molecules are added to 3THF, the geometrical properties of the compound change dramatically, this can be seen in plots of molecular geometries, electrostatic potential surfaces, and contour maps. New peaks appear in some coordination compounds which are not found in 3THF, otherwise peaks in 3THF disappear when 2Au adds to 3THF, the disappearance of the apex can be attributed to shielding procedure obtaining as a result to overlap between gold atoms and 3THF atoms. The highest apex in 3THF at approximately the density of state 3.2 under (-10 eV), but the highest apex in the coordination compound 3THF-2Sc demonstrate at approximately the density of state 4.4 under (-10 eV). The impurities (2Cr, 2Ni, 2Y, 2V, 2Sc, 2Pt, 2Au and 2Co) lead to dramatic change in the values of band gaps it change from the range of insulators to the range of semiconductors. Addition impurities (2Cr, 2Ni, 2Y, 2V, 2Sc, 2Pt, 2Au and 2Co) to 3THF make the values of ionization potential low, this can deem an improvement in the electronic properties of complexes compounds as compared with 3THF. 3THF-2Au has the lowest hardness value of about (1.0573 eV), so it has the highest value of softness, also this due to the inverse relationship between hardness and softness. The values of electronegativity for all coordination complexes nanoclusters (3THF-Metal) larger than the value of electrophilicity of 3THF, one can say addition the impurities (2Cr, 2Ni, 2Y, 2V, 2Sc, 2Pt, 2Au and 2Co) to 3THF lead to increase the values of electrophilicity. The (ligand-metal) 3THF-2V has the highest polarizability value, which is around (377.3503 a.u), this indicates that the 3THF -2Y coordination complex has the most vitality and activity.

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