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Accomplishment the Geometrical and Finding the Electronic features for (3B5)Ag, (3B5)Cd, (3B5)Cr, (3B5)Cu, (3B5)Mo, (3B5)Nb, (3B5)Ni and (3B5)Zn by Utilizing The Quantum Computational method DFT at LanL2Dz and LanL2MB basis sets

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Abstract:

This study Density functional theory method have been utilized in order to accomplish the electronic properties and diagnosis the ligand-metal nanoclusters $(3B_5)Ag$, $(3B_5)Cd$, $(3B_5)Cr$, $(3B_5)Cu$, $(3B_5)Mo$, $(3B_5)Nb$, $(3B_5)Ni$ and $(3B_5)Zn$ through sophisticated algorithms in Gaussian 09, Gauss-view 05 programs. Density of states of all coordination complexes nanoclusters in this treatise have been accomplished by using Gausssum 03 program. The characterstics molecular geometry of the ligands-metals nanoclusters, electrostatic potentials (ESP), contour density maps, diagnostics by infrared spectra (IR), Density of states (DOS), HOMO energy, LUMO energy, SOMO energy, Energy gap (E_g), ionization potential (I.P), electron affinity (E.A), dipole moment in (Debye) and the polarizability in (a.u). Photos of electrostatic potentials and contour maps demonstrate that the electronic charges assemble around some atoms, but disappear around other atoms. Diagnostic by IR shows the active regions and the wave numbers in (cm^{-1}) unit that correspond to the suitable bond lengths and wavelengths. Density of states schematics clarifies entity two types of orbitals alpha and beta in the coordination complexes nanoclusters $(3B_5)Cd$, $(3B_5)Cr$, $(3B_5)Mo$, $(3B_5)Ni$ and $(3B_5)Zn$, but only alpha orbitals in the coordination complexes nanoclusters $(3B_5)Ag$, $(3B_5)Cu$ and $(3B_5)Nb$. (Energy of HOMO and LUMO) and Energy gap (E_g) table summarizes presence two types of materials, semiconductors and insulator, only the coordination compolexes nanocluster $(3B_5)Cu$ has insulator properties. It has energy gap approximately (6.775 eV), but the other coordination complexes nanoclusters have semiconductor energy gap. Ionization potential and electron affinity table summarizes strength of donor and acceptor. Dipole moment table demonstrates that is no zero values of the dipole moment, because all coordination complexes nanoclusters in this treatise are heterogeneous, i.e. each one of them possess two types of atoms Boron atom and the metal atom. The maximum value of the average polarizability is for the coordination complex nanocluster $(3B_5)Nb$, which pretty much equal to (374.2 a.u), hence this coordination complex nanocluster is the maximum activity among the paradigms in this treatise. All coordination complexes nanoclusters has the point group symmetry (C_{2v}/C_1).

Key word: ***DFT, DOS, SOMO, Symmetry, Polarizability, Electrostatic Potential, Energy gap.***

Introduction:

Density Functional Theory (DFT) is a quantum computational method utilizes quantum physics and quantum chemistry to accomplish the geometrical structure (at the ground state) for many molecular systems by utilizing sophisticated algorithms in the Gaussian 09 software(Assadi & Hanaor, 2013). DFT utilizes the electron density ρ(r) rather than the wave function, so DFT uses functionals (which is a functions to other functions) (Oftadeh et al., 2011). Many functionals and approximations are utilized for improving the calculations of DFT, the functionals like exchange and correlation functionals and the approximations like Generalizes Gradient Approaches (GGA), Local Density Approaches (LDA) and Local Spin Density Approaches(Simons, 2000). DFT needs many basis sets so as to make the calculations have more accuracy, those basis sets like, 3-21G, LanL2DZ, LanLMB, and the hybrid functional (B3LYP). Basis sets are functions specialized to orbits with accordance to the molecular orbital theory, in which the molecular orbitals originate from the linear combination of the atomic orbits, each orbital can be described by one wave function. Alex Becke suggested (B3LYP) in (1993) in order to express the correlation exchange energies. Geometrical optimization procedure is utilizing all the approximations in order to make the geometrical structure the best. Nopel prize in chemistry donates to Walter Kohn and John Pople in (1998) for making huge improvements in DFT computations by employing quantum chemistry ideas (Tomberg, 2020).

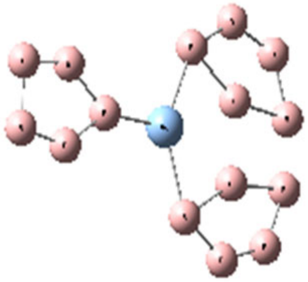
Coordination complex contains ligand and metal. The ligand typifies atom or assemble of atoms or a molecule can donate electrons to d orbital in transition metallic atom, hence the ligand plays a donor role, but the transition metallic atom will play acceptor role in the coordination complex. The bond which originate in the coordination complex is named coordination bond (Hauser, 2004). The coordination complex does not obey the traditional theories of covalence, but it obey Warner theory. Warner in (1893) suggested the metals have two sorts of covalence, the first is the oxidation case and the second is the coordination number (Lawrance, 2013). The coordination complexes are considered very important in many applications in number of different branch of knowledge such as medicine, pharmacy, biology and agricultural geometry. Haemoglobin, B12 vitamin and chlorophyll are well-known examples to the most important coordination complexes. The oxygen is carried from lungs to the tissues of human through haemoglobin. The nervous system and brain in human body need B12 vitamin. The chlorophyll is very necessary for plants, it play basic role in photosynthesis (Porterfield, 2013).

Results and Discussion

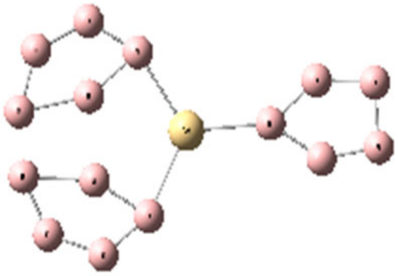
Molecular Geometry

One of the most important factors for describing the molecules that own single bonds is the repulsion among electrons. The repulsion has relationship with number of electron pairs around the central atom. The repulsion ought to be at the minimum value, and the ideal composition can get with dependence on the electrons that surround the central atom. In other words, it can be assert that the optimum possible composition of the molecule includes number of electrons around the central atom, the electrons must put in the orbits in which it is in directions make the repulsion at the lowest value. The minimum value of the energy is the standard which determine the molecular geometry (Gey, 1995). Molecular geometry of the coordination complexes nanoclusters $(3B_5)$Ag, $(3B_5)$Cd, $(3B_5)$Cr, $(3B_5)$Cu, $(3B_5)$Nb, $(3B_5)$Ni and $(3B_5)$Zn .

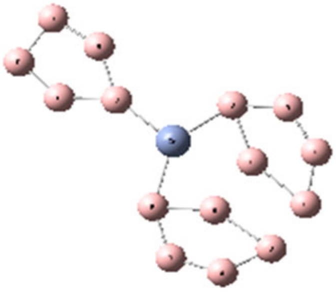
Figure (1) depicts the molecular structures of coordination complexes nanoclusters under the treatise, this molecular geometries obtain by the geometry optimization procedure. The atoms take the optimum locations after submitting the geometrical optimization, these positions appear the coordination complex nanocluster at the best values of the bond angles, dihedral angles and bond lengths. Making a comparison



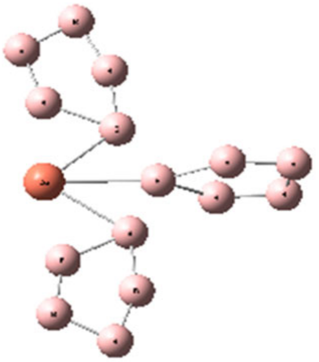
(3B$_5$)Ag



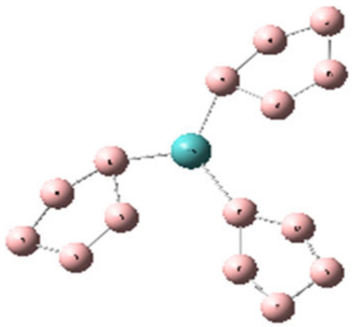
(3B$_5$)Cd



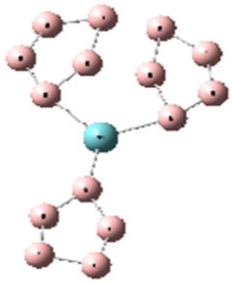
(3B$_5$)Cr



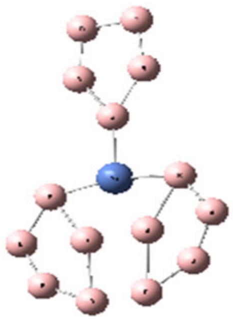
(3B$_5$)Cu



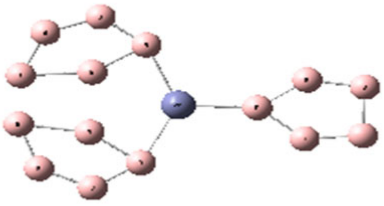
(3B$_5$)Mo



(3B$_5$)Nb



(3B$_5$)Ni



(3B$_5$)Zn

Figure (1) Molecular geometry of the coordination complexes nanoclusters (3B5)Ag, (3B5)Cd, (3B5)Cr, (3B5)Cu, (3B5)Mo, (3B5)Nb, (3B5)Ni and (3B5)Zn

between $(3B_5)Cd$ and $(3B_5)Cu$ shows apparently that the geometrical parameters are different in those two ligand-metal nanoclusters. The five atom boron rings in the ligand-metal nanocluster that contain copper $(3B_5Cu)$ arrange one close to other as compared with the ligand-metal nanocluster that has cadimium $(3B_5Cd$. Several physical and chemical parameters impact to the molecular geometry of the coordination complex nanocluster just like hybridization procedure, exclusion principle for Pauli and magnetic properties, According to those three factors the electrons can put in some orbitals, inversely the electrons may be prohibited to occupy other orbitals.

Electrostatic Potential (ESP)

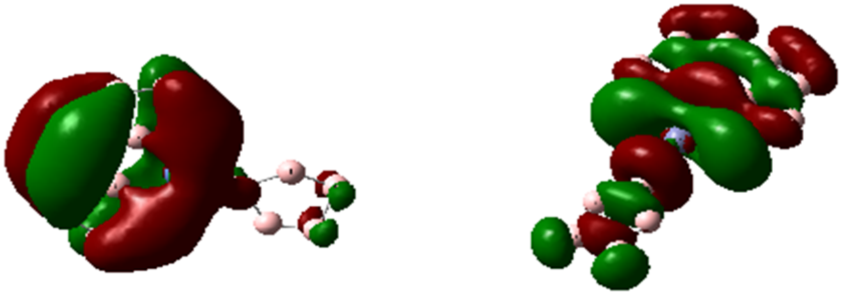
Through visualizing electrostatic potential surfaces the electrostatic energy maps will be clear, it demonstrate the charge distributions maps about the atoms in the molecule, it can be said that, it depict zones of existence the electrons. Each electron moves in the electrostatic field that the other atoms in the molecule (core field) create, which utilize Hamilton of one electron. The corresponding wave function solutions can be gotten throughout the atomic orbitals combination approximation. HOMO, LUMO and SOMO surfaces can be achieved through the order MOs in Gauss View 05 program after finishing the geometrical optimization procedure. This procedure stops when stationary point at the potential surface is existed, at that time, the force resultant at every atom in the structure will be zero (equilibrium state) (Frisch et al., 2015). Electrostatic potential surfaces of the coordination complexes nanoclusters $(3B_5)Ag$, $(3B_5)Cd$, $(3B_5)Cr$, $(3B_5)Cu$, $(3B_5)Nb$, $(3B_5)Ni$ and $(3B_5)Zn$.

It can be apparently visualized that the electrostatic potential surfaces in figure (2) with the colors red and green around the atoms. One can observe clearly that impact of the addition metal atom to the electrostatic potential surface in ligand-metal nanocluster surface. The figure also gives distribution of electronic charges around the atoms in the coordination complexes in nanoscale. Simplified comparison of the pictures shows charge distribution of electronic charges about the atoms in the coordination complexes nanoclusters $(3B_5)Cd$, $(3B_5)Zn$ is semi-homogeneous, but in the ligand-metal nanoclusters $(3B_5)Cu$, $(3B_5)Nb$ and $(3B_5)Mo$ charge distribution concentrates around atoms of two five atoms boron rings, this happen because some physical and chemical procedures just like symmetry and hybridization. When an atom in boron in p orbital translate to available d orbital in Cr or Zn, the atomic orbitals p and d may combine together to originate molecular orbital of the type pi (π) or delta (δ). HOMO, LUMO picture depict diffusion of the electronic density of the wave functions. Sign of wave function is very important, it determines positions of atoms in the coordination complexes nanoclusters in the coordinate-plane, but the probability of foundation of the electron can be described by the square of wave function. Dark red color in the electrostatic potential surface denotes to the negative partition of the wave function, but the green color in the electrostatic potential surface refers to the positive partition of the wave function.

$(3B_5)$Ag **$(3B_5)$Cd**

$(3B_5)$Cr **$(3B_5)$Cu**

$(3B_5)$Mo **$(3B_5)$Nb**

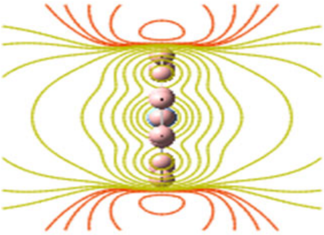


$(3B_5)$Ni **$(3B_5)$Zn**

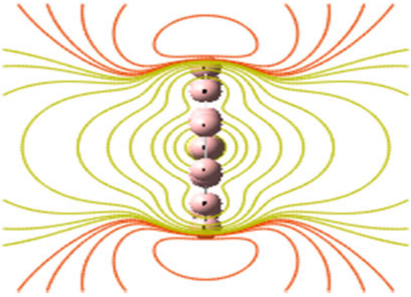
Figure (2) Electrostatic potential (ESP) for (3B5)Ag, (3B5)Cd, (3B5)Cr, (3B5)Cu, (3B5)Mo, (3B5)Nb, (3B5)Ni and (3B5)Zn

Contours

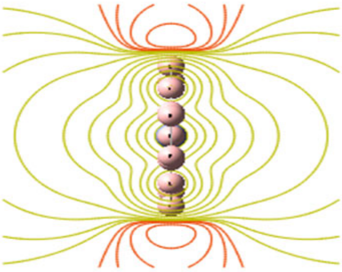
Many of problems in solid state physics especially the problems that involve to band theory and lattice vibration can be interpret depending on idea of reciprocal lattice, i.e. the reciprocal space, and because of the reciprocal space is very large, the scientist Brillion could division the space in to zones surround one another. The first zone that surround one lattice point is called first Brillion zone. The region which surround the first Brillion zone is called second Brillion zone, so on. Contour maps can stand for Brillion zone. Also Fermi surface shape can be detected by the closed curves engineering of energy (Ali et al., 2016). Contour maps of the coordination complexes nanoclusters $(3B_5)$Ag, $(3B_5)$Cd, $(3B_5)$Cr, $(3B_5)$Cu, $(3B_5)$Nb, $(3B_5)$Ni and $(3B_5)$Zn .



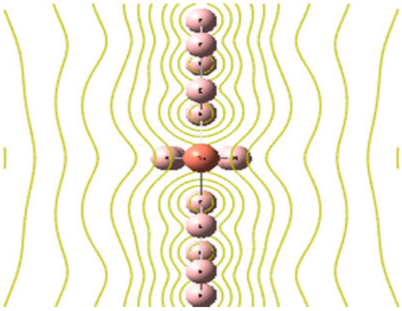
$(3B_5)$Ag



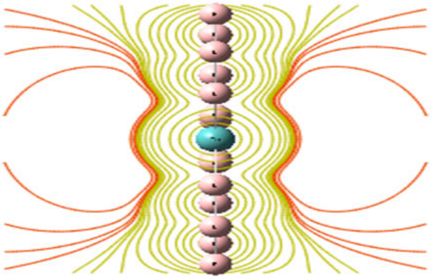
$(3B_5)$Cd



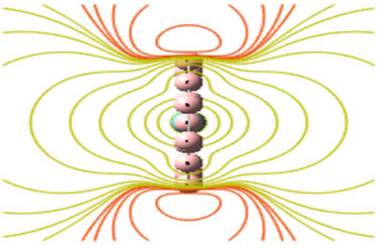
$(3B_5)$Cr



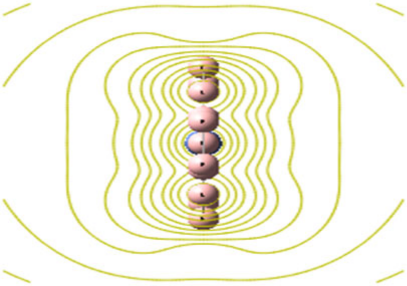
$(3B_5)$Cu



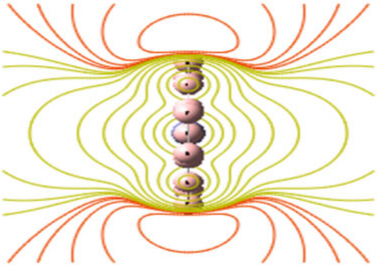
$(3B_5)$Mo



$(3B_5)$Nb



$(3B_5)$Ni



$(3B_5)$Zn

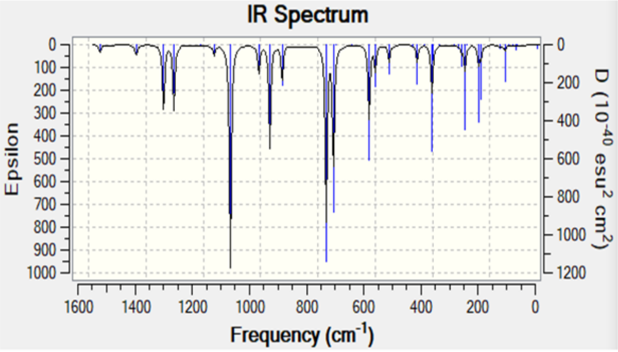
Figure (3)Density of contour maps for (3B5)Ag, (3B5)Cd, (3B5)Cr, (3B5)Cu, (3B5)Mo, (3B5)Nb, (3B5)Ni and (3B5)Zn

Figure (3) gives apparent the distortions in maps of contours density and charge transfer from p orbital in the ligands (B_5 rings) to the metal atoms (Ag , Cd , Cr , Cu , Mo , Nb , Ni and Zn). One can visualize that charges density and contour maps distribution around the atoms and B_5 rings vary according to the type of impurity. Contour maps distribution in ($3B_5$)Zn and ($3B_5$)Nb concentrate clearly around B_5 rings in the ligand-metal nanocluster. Charge density in ($3B_5$)Mo distribute around Molybdenum and some boron atoms in the five atoms rings with high concentration as compared with other coordination complexes nanoclusters. Charge distribution of electron charges in the ligand metal nanoclusters ($3B_5$)Cu and ($3B_5$)Ni is less density as compared with all other coordination complexes nanoclusters under this treatise. The variation in the charge density distribution around atoms and B_5 rings take place as a result to some parameters and properties just like geometrical parameters and topological properties. The electrons movement in contour circles is restricted, but near zone boundaries the contour energy curves vanish. When corners of first Brillion zone perfectly fill, there is no electron enters the second zone unless the electron has energy make it able to cross the prohibited zone between first and second Brillion zone.

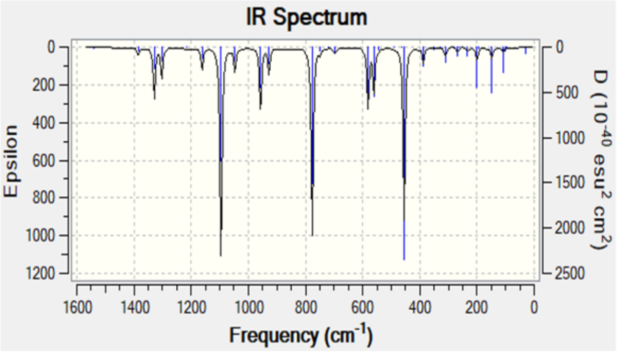
Infrared spectra (IR)

In solid state physics and chemistry infrared spectra can be utilized to examine the substances. In all substances solids, gases and liquids IR spectra can get experimentally through spectrometers. One of the most important devices for getting IR spectra is (FTIR). Theoretically infrared spectra can result throughout programs just like Gaussian 09 program. The molecular system can vibrate in many ways, every way is called vibration mode. Through IR spectra it can examine vibrational frequencies. The vibrations may be symmetric (atoms with the same type) or asymmetric (atoms with different type). Stretching oscillation gets when atoms oscillate in the same phase, but non-stretching oscillation results when the atoms vibrate in different phase(Alwan, 2020). Infrared spectra of the coordination complexes nanoclusters ($3B_5$)Ag, ($3B_5$)Cd, ($3B_5$)Cr, ($3B_5$)Cu, ($3B_5$)Nb, ($3B_5$)Ni and ($3B_5$)Zn.

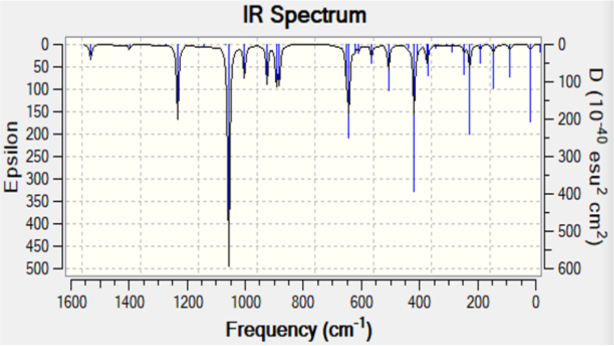
Figure (4) summarizes infrared spectra schematics which demonstrates active regions in the coordination complexes nanoclusters under the treatise. Making comparison between the ligand-metal nanoclusters ($3B_5$)Ag and ($3B_5$)Mo shows that the coordination complex nanocluster that implicit Ag has approximately more than eleven clear apexes, that apexes signifies to presence of bonds (B-B) and (B-Ag) correspond certain wave numbers, but the coordination complex nanocluster that implicit Mo has approximately five apparent apexes at certain wave numbers, that apexes signifies to presence of bonds (B-B) and (B-Mo). Generally in the schematics of IR spectra $x-$ axis contains wave number in cm^{-1} (reciprocal centimeter) and $y-$ axis represents the intensity in km/mole unit. Simplified comparison among samples in this study demonstrates ($3B_5$)Cu has the highest apex at the intensity (1700 km/mole) corresponding to the wave number approximate (1300 cm^{-1}), ($3B_5$)Mo has the highest apex at the intensity (3700 km/mole) corresponding to the wave number approximate (1300 cm^{-1}), but ($3B_5$)Nb has the highest apex at the intensity (625 km/mole) corresponding to the wave number approximate (1075 cm^{-1}). Wave number refers to number of atoms to each centimeter. In the coordination complex nanocluster ($3B_5$)Cu the formulated bonds of the type (B-B) and (B-Cu), but in the coordination complex nanocluster ($3B_5$)Nb the formulated bonds of the type (B-B) and (B-Nb).



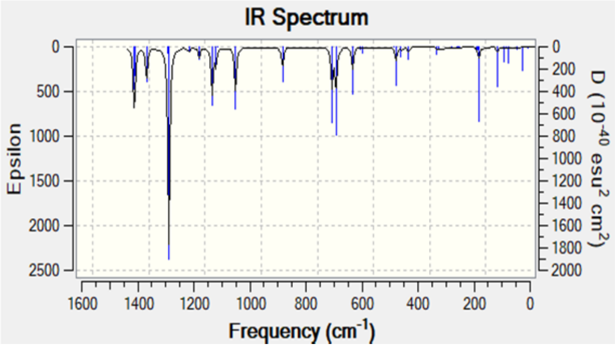
(3B$_5$)Ag



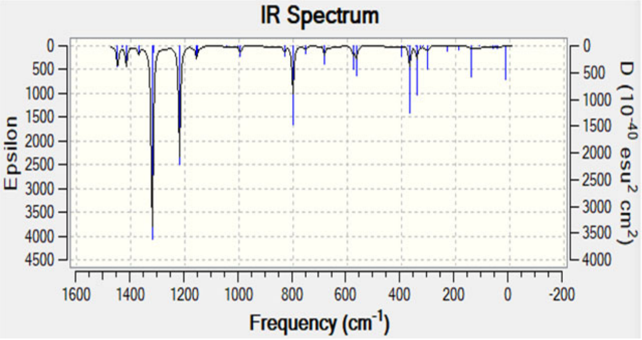
(3B$_5$)Cd



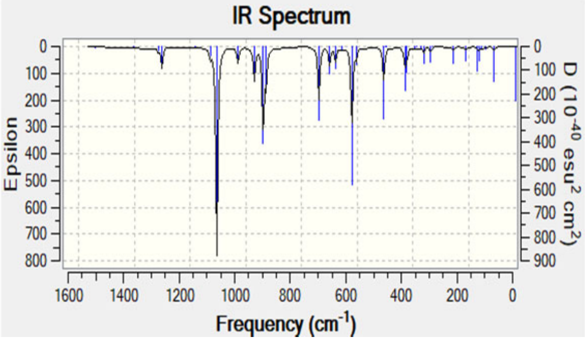
(3B$_5$)Cr



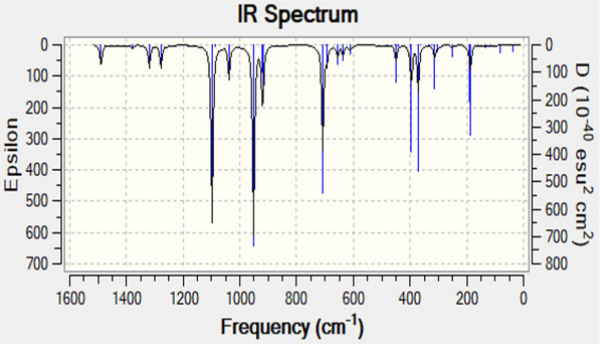
(3B$_5$)Cu



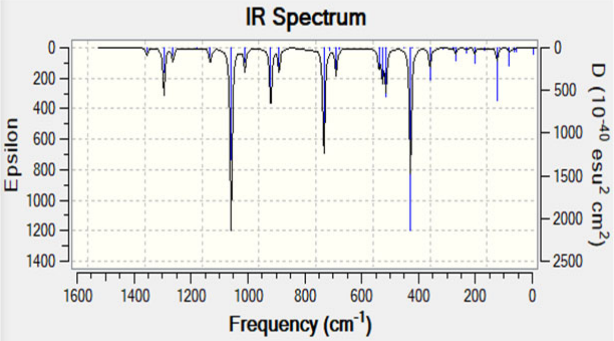
(3B$_5$)Mo



(3B$_5$)Nb



(3B$_5$)Ni



(3B$_5$)Zn

Figure (4)Infrared spectra schematics for (3B5)Ag, (3B5)Cd, (3B5)Cr, (3B5)Cu, (3B5)Mo, (3B5)Nb, (3B5)Ni and (3B5)Zn

Electronic states Energy Gap (E_g)

The energy which the electron possess at the highest occupied orbital of the molecular orbitals is called E_{HOMO}, but the energy which the electron possess at the lowest unoccupied orbital of the molecular orbitals is called E_{LUMO}, the energy difference between them is named the energy gap (E_g). Band energy gap is of the very important quantities in physics, through energy gap it can be distinguish among the substance if they are conductors, semiconductors, semi-metals or insulators. According to band theory there are two bands, one of them is valence band which is completely full with electrons, the other is conduction band, which is completely empty of electrons, there is region between those two bands, this region is called forbidden energy gap. Mathematically the energy gap (E_g) can be expressed as the equation (Adekoya et al., 2021)

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

Table (1) illustrates HOMO, LUMO energies and energy gaps for ($3B_5$)Ag, ($3B_5$)Cd, ($3B_5$)Cr, ($3B_5$)Cu, ($3B_5$)Mo, ($3B_5$)Nb, ($3B_5$)Ni and ($3B_5$)Zn

System	EHOMO(eV)	ELUMO(eV)	Eg(eV)
($3B_5$)Ag	**-6.0482388**	**-4.9198401**	**1.1283987**
($3B_5$)Cd	**-5.8466127**	**-4.7878716**	**1.0587411**
($3B_5$)Cr	**-6.2806122**	**-4.9497711**	**1.3308411**
($3B_5$)Cu	**-7.5224766**	**-0.7474587**	**6.7750179**
($3B_5$)Mo	**-4.1457156**	**-2.8744644**	**1.2712512**
($3B_5$)Nb	**-6.0098727**	**-5.0063679**	**1.0035048**
($3B_5$)Ni	**-6.4770684**	**-4.4891058**	**1.9879626**
($3B_5$)Zn	**-5.8389939**	**-4.786239**	**1.0527549**

Table (1) summarizes values of the physical quantities E_{HOMO} , E_{LUMO} and E_g of the coordination complexes nanoclosters under this treatise. The ligand-metal nanocluster ($3B_5$)Mo has the maximum value of E_{HOMO}, therefore the electrons will release from the orbits of this coordination complex nanocluster easier than the other coordination complexes nanoclusters. The ligand-metal nanocluster ($3B_5$)Cu owns the minimum value of E_{LUMO}, therefore the electrons will release from the orbitals of this coordination complex nanocluster, this paradigm accepts the electrons in the available orbitals easier than the other coordination complexes nanoclusters. One can make a simplified counter-posing among the ligand-metal nanoclusters under the treatise in order to deduce there are two types of coordination complexes nanoclusters, they may be semiconductors or insulator. All coordination complexes nanoclusters possess energy gap in the domain of semiconductors except the coordination complex nanocluster ($3B_5$)Cu which has energy gap in the domain of the insulators it is (6.7750179eV) . One can put it addition the impurity of copper in the center of the ligand-metal nanocluster ($3B_5$)Cu makes it behave as an insulator. The ligand-metal nanocluster ($3B_5$)Ag has energy gap approximately (1.12 eV) , this value closes to the value of energy gap of silicon. Studying energy gap characterstic has greater importance in the electronic applications, just like solar cells, making computer species just like processor and sensors.

Ionization potential and electron affinity

For atom or molecule, the ionization energy is the minimum energy for eliminating an electron from the gaseous atom or molecule at the stationary state. The eliminating electron in this case separates from the proton. So as to eliminate an electron from the orbital, the electron ought to have enough energy to overcome the binding energy. The electron affinity stands for the required energy to remove an electron from negative ion. Sometimes the electron affinity is called the zero ionization energy. If it is possible to add an electron to orbital easily in order to complete the configuration of the shell, here, the electron affinity will be relatively large, but the atoms that implicit closed principal shells or closed secondary shells in general have small electron affinity. According to Koopman theory ionization energy and electron affinity can be described in terms of energy of HOMO and energy of LUMO respectively (Mohammed L. Jabbar, 2020).

$$I.P = -E_{HOMO} \quad \dots \quad (2)$$

$$E.A = -E_{LUMO} \quad \dots \quad (3)$$

Table(2) reveales Ionization potentials (I.P) and electron affinities (E.A) for $(3B_5)$Ag, $(3B_5)$Cd, $(3B_5)$Cr, $(3B_5)$Cu, $(3B_5)$Mo, $(3B_5)$Nb, $(3B_5)$Ni and $(3B_5)$Zn

System	I.P(eV)	E.A(eV)
$(3B_5)$Ag	6.0482388	4.9198401
$(3B_5)$Cd	5.8466127	4.7878716
$(3B_5)$Cr	6.2806122	4.9497711
$(3B_5)$Cu	7.5224766	0.7474587
$(3B_5)$Mo	4.1457156	2.8744644
$(3B_5)$Nb	6.0098727	5.0063679
$(3B_5)$Ni	6.4770684	4.4891058
$(3B_5)$Zn	5.8389939	4.786239

Table (2) summarizes values of ionization potentials and electron affinity of the coordination complexes nanoclusters in this treatise. The ligand-metal nanocluster $(3B_5)$Mo has the lowest value of ionization potential among all coordination complexes nanoclusters in this study, the value here is (4.1457156 eV), one can assert that the electrons in this coordination paradigm need the minimum energy for breaking free the orbitals, that is to say, this ligand-metal nanocluster donates the electrons easier than other coordination paradigms. The coordination complex nanocluster $(3B_5)$Cu has the maximum value of ionization potential among all paradigms, hence, this coordination complex nanocluster need high ionization energy to become cation, but the coordination complex nanocluster $(3B_5)$Mo need the minimum ionization energy to become cation. The ligand-metal nanocluster $(3B_5)$Cu has the minimum electron affinity in this treatise, hence, the electrons in this coordination complex nanocluster need less energy to occupy empty orbits, the energy release from addition the electrons to LUMO. The electron affinity stands for a measure to the strength of donor. The ionization potential and electron affinity represent tremendously very important characterstics for determining another properties which is very beneficial in physics and chemistry, just like, hardness, softness, electronegativity and electrophilicity.

Dipole moment

The dipole consists of two poles separate their center determination displacement, those two poles dissimilar in the signs. The two poles may be electric poles positive and negative, also they are perhaps magnetic poles northern and southern, although there is no single magnetic pole, but there is two poles for each magnet. The simplified example to the dipole is the straight magnet. Electric dipole moment is a vector quantity, that is to say, electric dipole moment has value and direction. Let $\vec{\mu}$ stands for the electric dipole moment vector, q_i represents the resultant of sum of charges, and the quantity r_i denotes to the vector which represent locations of the charges, hence the electric dipole moment can be described mathematically by the equation below(Alwan et al., 2019) .

$$\vec{\mu} = \sum q_i \ r_i \qquad \dots \quad (4)$$

Table (3) appears dipole moments for $(3B_5)$Ag, $(3B_5)$Cd, $(3B_5)$Cr, $(3B_5)$Cu, $(3B_5)$Mo, $(3B_5)$Nb, $(3B_5)$Ni and $(3B_5)$Zn

System	Dipole moment (Debye)
$(3B_5)$Ag	1.0549
$(3B_5)$Cd	5.1885
$(3B_5)$Cr	0.4292
$(3B_5)$Cu	6.1246
$(3B_5)$Mo	4.3140
$(3B_5)$Nb	1.5096
$(3B_5)$Ni	1.4152
$(3B_5)$Zn	4.9697

The table (3) summarizes the numerical values of the electric dipole moment of the coordination complexes nanoclusterts under this treatise. The dipole moment typifies general measure to the properties, strength of the bond and the density of charge in chemical structure. The dipole moment gives information around the polarizability because it predict to the activity of ligand-metal nanocluster. The maximum value of electric dipole moment is for the coordination complex nanocluster $(3B_5)$Cu, it is (6.1246 Debye), and the minimum value of dipole moment is for the coordination complex nanocluster $(3B_5)$Cr, it is (0.4292 Debye). One can notice apparently that there is no zero values for dipole moment, the reason here, all coordination complexes nanoclusters in this treatise consist of two types of atoms ligand (Boron) and metal (Ag , Cd , Cr , Cu , Mo , Nb , Ni and Zn), therefore one can put it the electric dipole moment originates because of dissimilarity in the interaction atoms.

Polarizability

One of the most important quantities in order to know the characterstics of the substances is the electric polarizability. In another words the polarizability stands for the trend of charge distribution, just like the electrons for atom or molecule which leads to the distortion from the natural picture by applying external electric field so as to acquire electric dipole moment. The polarizability measures the linear response to the electron density with existence of infinite seminal electric field, which represent second order derivative with respect to the variation in energy. Mathematically it can be described by the equation below (Kassar, 2021).

$$\alpha = -\left(\frac{\partial^2 E}{\partial F_a \partial F_b}\right)_{a,b} = x, y, z \quad \dots (5)$$

If some molecules are plane and the other not, it is very beneficial to decide the polarizability quantities that are invariant in order to choose the coordinate-system. The average polarizability is calculated by the equation below (Griffiths, 2005).

$$< \alpha > = \left(\frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3}\right) \quad \dots (6)$$

The quantities α_{xx} , α_{yy} and α_{zz} typify the eigen values to the polarizability tensor.

Table (4) summarizes polarizabilities and average polarizabilities for $(3B_5)$Ag, $(3B_5)$Cd, $(3B_5)$Cr, $(3B_5)$Cu, $(3B_5)$Mo, $(3B_5)$Nb, $(3B_5)$Ni and $(3B_5)$Zn

System	α_{xx}	α_{yy}	α_{zz}	$< \alpha >$
$(3B_5)$Ag	**126.209**	**302.122**	**474.271**	**300.8673333**
$(3B_5)$Cd	**134.704**	**346.368**	**619.575**	**366.8823333**
$(3B_5)$Cr	**122.327**	**295.811**	**563.571**	**327.2363333**
$(3B_5)$Cu	**154.472**	**343.246**	**300.074**	**265.9306667**
$(3B_5)$Mo	**97.912**	**463.324**	**378.079**	**313.105**
$(3B_5)$Nb	**157.852**	**302.045**	**662.737**	**374.2113333**
$(3B_5)$Ni	**116.658**	**296.694**	**440.035**	**284.4623333**
$(3B_5)$Zn	**127.846**	**334.889**	**583.771**	**348.8353333**

Table (4), it can be seen the eigen values of polarizabilities α_{xx} , α_{yy} , α_{zz} and the average polarizability $< \alpha >$ for the coordination complexes nanoclusters in the treatise. The average polarizability of the ligand-metal nanocluster $(3B_5)$Nb is the maximum value among all coordination complexes nanoclusters $(3B_5)$-metal, (metal= Ag , Cd , Cr , Cu , Mo , Nb , Ni , Zn), hence the ligand-metal nanocluster $(3B_5)$Nb is the maximum vitality among $(3B_5)$-metal nanoclusters. But the coordination complex nanocluster $(3B_5)$Cu has the minimum value ligand-metal nanocluster, therefore $(3B_5)$Cu is the minimum vitality ligand-metal nanocluster. One can make a comparison among the coordination complexes nanoclusters with accordance to the eigen values of the polsarizability tensor, The highest value of α_{zz} is for the coordination complex nanocluster $(3B_5)$Cd, it is (619.575 a.u). The highest value of α_{yy} is for the ligand-metal nanocluster $(3B_5)$Mo, it is (463.324 a.u). The highest value of α_{xx} is for the coordination complex nanocluster $(3B_5)$Nb, it is (157.852 a.u). The polarizability is very important property in physics, it gives information about the internal structure and the electric dipole moment for the coordination complexes nanoclusters without holding calculations. Polarizability characterstic is very beneficial in the nonlinear optics science.

Symmetry

The symmetry takes place around surface, centerpiece or point. The procedures of symmetry are three, rotation, reflection and inversion. The rotation operation require knowledge number of times in which the geometrical figure repeat itself during rotation complete cycle (2π), The number of times is named number of folds. The geometrical figure has reflection symmetry about any symmetry plane if there is no change in geometrical figure after reflection from this plane. The inversion symmetry takes place when a geometrical figure rotates with certain angle and reflect about straight line at the same time throughout point on it, the geometrical figure will take it's location place (Talib & Alwan, 2022).

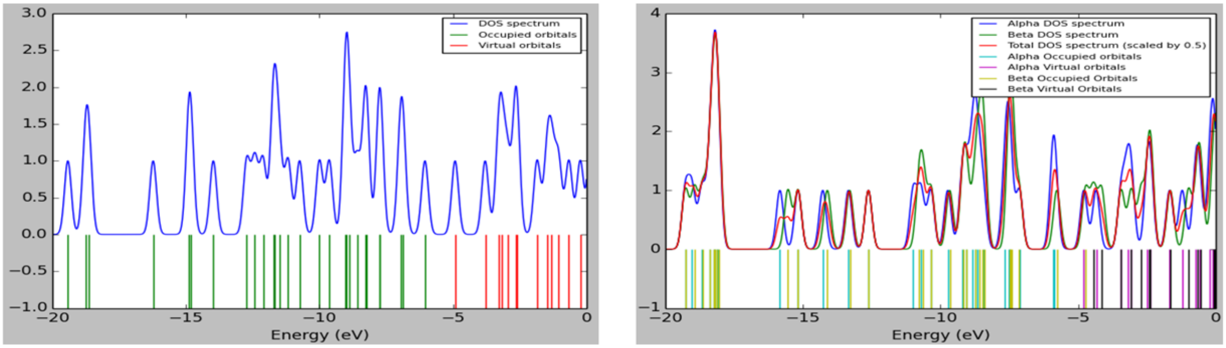
Table (5) appears point group symmetries for $(3B_5)$Ag, $(3B_5)$Cd, $(3B_5)$Cr, $(3B_5)$Cu, $(3B_5)$Mo, $(3B_5)$Nb, $(3B_5)$Ni and $(3B_5)$Zn

System	Point group symmetry
$(3B_5)$Ag	C_{2v}/C_1
$(3B_5)$Cd	C_{2v}/C_1
$(3B_5)$Cr	C_{2v}/C_1
$(3B_5)$Cu	C_{2v}/C_1
$(3B_5)$Mo	C_{2v}/C_1
$(3B_5)$Nb	C_{2v}/C_1
$(3B_5)$Ni	C_{2v}/C_1
$(3B_5)$Zn	C_{2v}/C_1

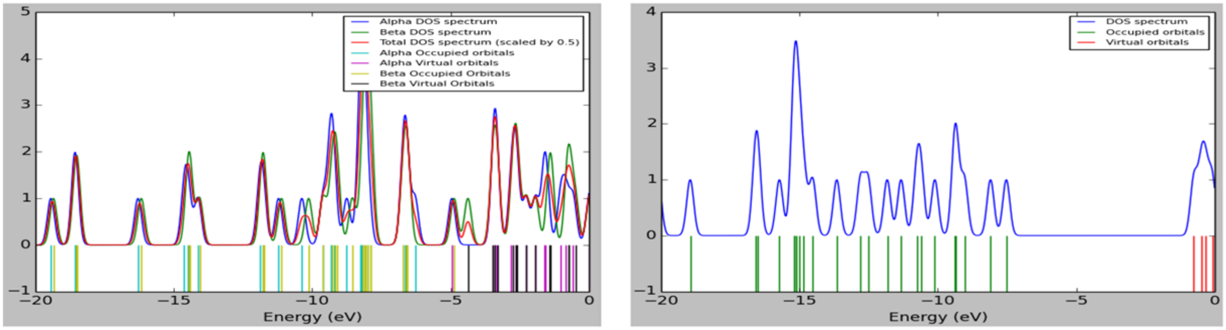
Table (5) demonstrate kind of point group symmetry of the coordination complexes nanoclusters in this study. All ligand-meal nanoclusters in this treatise has one type of point group symmetry, the symmetry is (C_{2v}/C_1). This point group symmetry kind denotes to that the symmetry in all coordination complexes nanoclusters reflect the coordination complex nanocluster through plane contains principal centerpiece and also all coordination complexes nanoclusters have plane of mirror plane (σ_v), so all ligand-metal nanoclusters have the symmetry C_n , that is to say, the symmetry happens through $(360^o/n)$, hence the coordination complexes nanoclusters repeat itself throughout (360^o), because they have the symmetry (C_1). In another phrase this symmetry operation reflect the coordination complexes nanoclusters through planes contains major axis which is the vertical planes, all ligand-metal nanoclusters have two vertical planes of the symmetry.

Density of States (DOS)

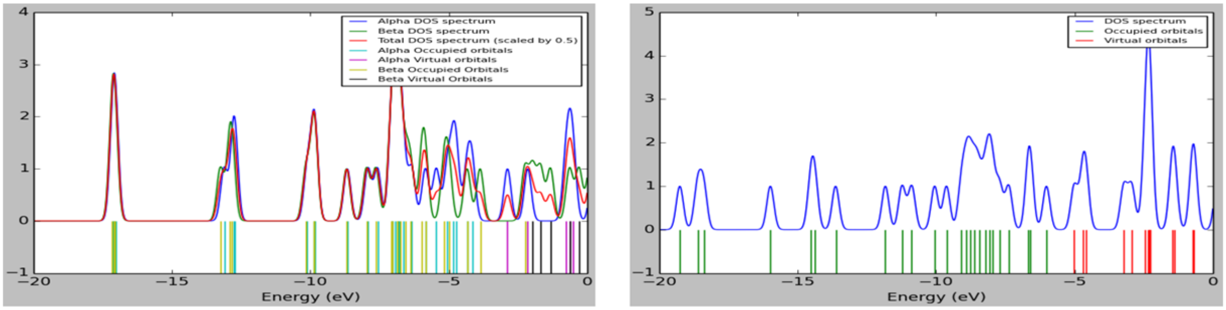
Number of states for the energy unit is called the density of states. Understanding the notion of density of states aid to understand and interpret many of physics phenomena. Knowledge of density of state at Fermi level has greater importance in the study of metals characterstics. In the density of states calculations had been chosen surface with constant energy has value ranges between determined value and the same value plus the change in this value. Also it had been chosen volume section in the wave number vector space. So density of state can be defined as the number of electronic quantized states that will be available for every interval of energy range (certain range of energy swing between two values), here, it ought to take in consideration each state can take only two electrons (Shwya et al., 2020) Density of states for the coordination complexes nanoclusters $(3B_5)$Ag, $(3B_5)$Cd, $(3B_5)$Cr, $(3B_5)$Cu, $(3B_5)$Nb, $(3B_5)$Ni and $(3B_5)$Zn .



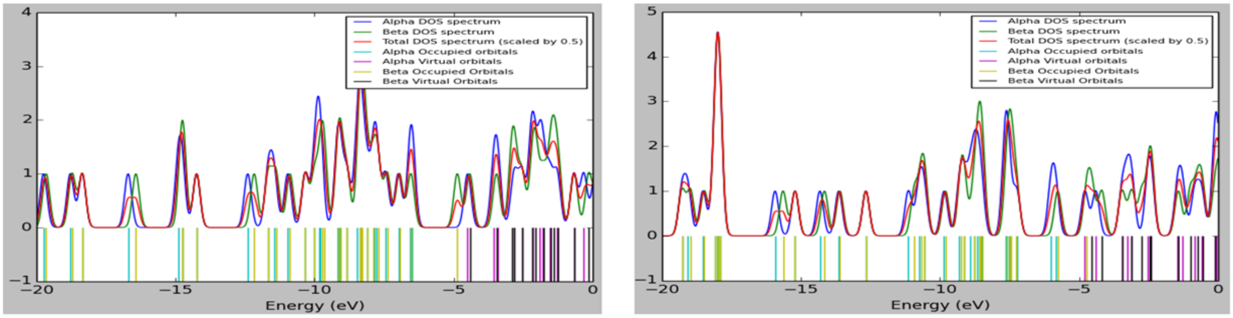
(3B$_5$)Ag (3B$_5$)Cd



(3B$_5$)Cr (3B$_5$)Cu



(3B$_5$)Mo (3B$_5$)Nb



(3B$_5$)Ni (3B$_5$)Zn

Figure (5)Density of state charts for (4C4)Sc, (4C4)Cr, (4C4)Sc, (4C4)Mo, (4C5)Ni,(4C5)Fe, (4C5)Sc and (4C5)Mo

Throughout the figure (5) demonstrate density of states diagrams for some coordination complexes nanoclusters have two types of orbitals alpha (α) and beta (β), but the others have only alpha (α)

orbitals. The ligand-metal nanoclusters ($3B_5$)Cd, ($3B_5$)Cr, ($3B_5$)Mo, ($3B_5$)Ni and ($3B_5$)Zn have two types of orbitals alpha (α) and beta (β). The ligand-metal nanoclusters ($3B_5$)Ag, ($3B_5$)Cu and ($3B_5$)Nb have only alpha (α) orbitals. The coordination complexes nanoclusters that have two type of orbitals alpha and beta have orbitals with open shell systems, that is to say, the occupied orbital will be SOMO, i.e. the occupied molecular orbital will be single. In this single orbital, it cannot put more than one electron in the orbital. The coordination complexes nanoclusters ($3B_5$)Cd, ($3B_5$)Cr, ($3B_5$)Mo, ($3B_5$)Ni and ($3B_5$)Zn behave as an anti-ferromagnetic materials because they have SOMO orbital, in this kind of materials there is no two electrons in the orbital, and the minor shell (d) has magnetic moments or spins in the solid state with the same scalar, but in the opposite direction to the neighboring magnetic moments, in which the magnetic moments resultant of the anti-ferromagnetic materials ought to equal to zero. DOS schematics depict number of states that can be occupied by electrons and how the electrons exist in the orbitals, the electrons will occupy new locations in order to get more stability ligands-metals nanoclusters. Also one can visualize energy gaps of the coordination complexes nanoclusters throughout the schematics of DOS, the energy gap stands for the energy difference between conduction band (E_{LUMO}) and valence band (E_{HOMO} or E_{SOMO}). The highest apex in the density of states illustrations is for the coordination complex nanocluster ($3B_5$)Zn at (4.6 arbitrary unit) under around approximately (-18 eV).

Conclusions

The atoms take the optimization positions after achieving the geometrical optimization, these positions demonstrate the coordination complex nanocluster at the best values of the geometrical parameters. Two types of orbits alpha and beta will originate in some coordination complexes nanoclusters, but only alpha orbits will generate in the others as a result to the linear combination between p orbitals Boron and d orbitals in the metal. According to contour maps charge density distribution in some coordination complexes nanoclusters are approximately regular, but in the others will be irregular. According to IR diagnostics kind of impurity leads to dissimilarity active groups correspond to determined wavelengths will demonstrate in the coordination complexes nanoclusters. The impurity of copper in the center of the ligand-metal nanocluster ($3B_5$)Cu leads to behavior of the coordination complex nanocluster ($3B_5$)Cu as an insulator, it has the energy gap approximately (6.775 eV), but the other coordination complexes nanoclusters behave as semiconductors, the energy gap domain of them between approximately (1.0035 eV) for ($3B_5$)Nb and (1.9879 eV) for ($3B_5$)Ni, this property is very important in the electronic devices. The coordination complex nanocluster ($3B_5$)Mo has minimum value of ionization energy, hence it needs the lowest energy to break free the orbitals, so it can donate the electrons easier than other coordination complexes nanoclusters in this research. The electrons in the coordination complex nanocluster ($3B_5$)Cu need less energy to occupy empty orbits, the energy release from addition the electrons to LUMO because it has the lowest value of electron affinity, it is pretty much (0.7474 eV). The coordination complex nanocluster ($3B_5$)Cu possess the maximum value of electric dipole moment, it is (6.1246 Debye), this appear effect of copper as impurity as compared with other impurities. All ligand-metal nanoclusters have plane of mirror plane (σ_v) and repeat itself during (2π), i.e. repeat itself each one cycle. The highest value of the polsarizability tensor α_{zz} is for the coordination complex nanocluster ($3B_5$)Cd, the highest value of α_{yy} is for the ligand-metal nanocluster ($3B_5$)Mo, but the highest value of α_{xx} is for the coordination complex nanocluster ($3B_5$)Nb. The coordination complexes nanoclusters ($3B_5$)Cd, ($3B_5$)Cr, ($3B_5$)Mo, ($3B_5$)Ni and ($3B_5$)Zn behave as an anti-ferromagnetic materials, i.e. there is no two electrons in the orbital.

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