International Journal of Physics and Applications

E-ISSN: 2664-7583
P-ISSN: 2664-7575
Impact Factor (RJIF): 8.12
IJOS 2025; 7(2): 147-155
© 2025 IJPA
www.physicsjournal.in
Received: 02-06-2025
Accepted: 05-07-2025

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Studying the electronic properties for the interactions between (V_6C_6), $(Ni_4C_4)/(CO_2)_2$ with 4S and $(SiO)_2$ through DFT

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DOI: https://www.doi.org/

Abstract
Density functional theory (DFT) at B3LYP level, ground state energy and the basis set 6-31G have been employed with sophisticated algorithms in Gaussian 09 package to find out the following merits: the molecular geometry, electrostatic potential (ESP), contour maps, infrared spectra (IR), density of states (DOS), the electronic states HOMO and LUMO, the energy gap (E_g), dipole moment, average polarizability, and point group symmetry for the nanomaterial structures structures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$. The pictures of electrostatic potential depict charge exchange phenomena between vanadium atoms and silicon atoms in the interaction (V_6C_6)-$(SiO)_2$. The contour density maps demonstrated the active regions in the molecular structure when (V_6C_6) interacts with four sulfur atoms, the pictures of contours disclose the regions of interactions. New peaks demonstrated in the IR diagrams denote to new bonds result by means of the interactions, but sometimes the peaks disappear after the interaction because of shielding procedure. Diagrams of DOS point out that new energetic states can be occupied by electrons after the interactions between (V_6C_6), $(Ni_4C_4)/(CO_2)_2$ on the one hand, with 4S, $(SiO)_2$ on the other hand. The values of the energy gap all in the domain of the energy gap of semiconductors, this make the nanomaterials under study acquire an importance in the creation of solar cells and photoelectric cells. All nanomaterial structures have non-zero dipole moment because they are hetronuclear nanostructures. The interactions leads to increasing values of average polarizability. Two kinds of point group symmetries have been demonstrates C_1 and C_2/C_1.

Keywords: DFT, energy gap (E_g), infrared spectra (IR), symmetry, density of states

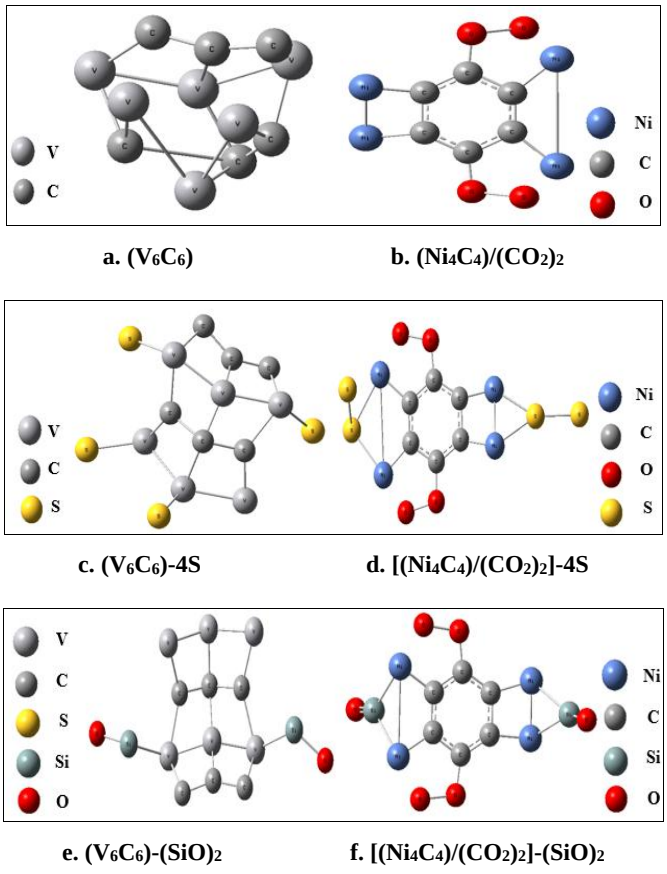
Introduction
Density functional theory (DFT) is a method for accomplishing the electronic properties, molecular structure, and the surfaces for atoms, molecules, semiconductors and nanoclusters [1]. This method is widely emloyed in material science and solid state physics [2]. DFT method employs the electron density in state the wave function. It implies that the electron density depends only on spatial coordinates, without considering how the electrons will be presence in the system [3]. The wave function is supposing one spin coordinate and 3N variables, three dimensional coordinates, one coordinate to the spin, by presupposition the positions of the nuclei be fixed [4]. Density functional theory is regarded as one of the most popular methods in computational physics and chemistry [5]. DFT is a method which is utilized to find out the solution of the Schrodinger equation for a system of many particles [6]. In solid state physics, most theoretical calculations agree well with the data which obtained by the experiments in the labs [7]. The term density functional theory was suggested by the means of the electron density function was employed in the calculations rather than the wave function [8]. Density functional theory was introduced in the 1960s in a two foundational papers by Hohenberg-Kohn in 1964 and Kohn-Sham in 1965. Density functional theory's precursor is Thomas-Fermi model which was presented in 1927 [9]. Among the approximations that had been employing in DFT are the Generalized Gradient Approximation (GGA), Local Density Approximation (LDA), and Local Density Spin Approximation (LDSA) [10]. Density functional theory achieves the molecular systems throughout usage a quitessential algorithms in the Gaussian 09 package and Gauss View 05 program. DFT requires the usage of sufficient basis sets to get more accurate calculations [11]. The basis sets importance comes from it describes the orbitals by a functions in which the atomic orbitals are

combining linearly with accordance to the molecular orbital theory. Alex Becke had presented the hybridization functional (B3LYP) in 1993 so as to exress on the correlation-exchange energies [12]. John Pople and Walter Kohn deserved Nople prize in chemistry by means of they were developing the calculations of DFT depending on the thoughts of quantum chemistry [13]. The goal of the study is to find out organic complex nanomaterial structures have merits make it acquire a significance in the manufacture of the electronic devices such as nanosensors and gas trapping. Also the treatise seeks on the possibility of utilization these organic complex nanomaterials as an electrochemical catalysis.

Result and discussion

Molecular geometry

The molecular geometry may be described through the method of configuration of atoms in the molecular systems. The molecular structure is a crucial characteristics by means of it yields an advantageous informations without holding calculations, the properties just like polarizability [14]. The molecular structure composes of atoms which links to each other to appear as a one particle. In general when the atoms draw near one another, it may be ionic bond originates, or covalent bond emerges, or perhaps no bond generate and in this case the system will be non-stable [15]. The molecular geometry of the nanomaterial structures (V_6C_6), (Ni_4C_4)/(CO_2)$_2$, (V_6C_6)-4S, [(Ni_4C_4)/(CO_2)$_2$]-4S, (V_6C_6)-(SiO)$_2$ and [(Ni_4C_4)/(CO_2)$_2$]-(SiO)$_2$ had been accomplished by utilization the density functional theory throughout sophisticated algorithms in Gaussian 09 program, 6-31G basis set and the hybrid functional B3LYP.



a. (V_6C_6) **b. (Ni_4C_4)/(CO_2)$_2$**

c. (V_6C_6)-4S **d. [(Ni_4C_4)/(CO_2)$_2$]-4S**

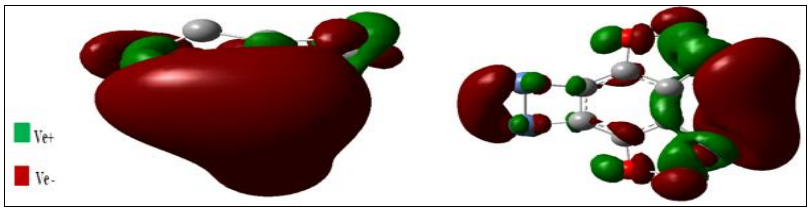
e. (V_6C_6)-(SiO)$_2$ **f. [(Ni_4C_4)/(CO_2)$_2$]-(SiO)$_2$**

Fig 1: Molecular structure for the nanostructures (V_6C_6), (Ni_4C_4)/(CO_2)$_2$, (V_6C_6)-4S, [(Ni_4C_4)/(CO_2)$_2$]-4S, (V_6C_6)-(SiO)$_2$ and [(Ni_4C_4)/(CO_2)$_2$]-(SiO)$_2$.

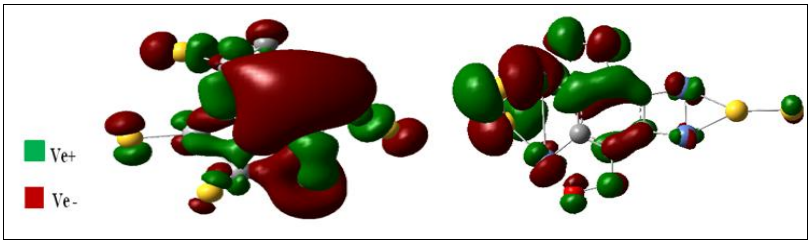
Figure (1) demonstrates nickel atoms with light blue color, carbon atoms with lead color, oxygen atoms with red color, vanadium atoms with rationally light lead color, sulfur atoms with yellow colorand silicon atoms with light turquoise color. When the organic complex nanostructure (V_6C_6) interacts with sulfur atoms, the sulfur atoms have a tendency to acquire electrons by means of possess two places in two orbitals can be occupied by two electrons, each 3p orbital can take one electron, but the vanadium has two electrons in the orbital 4s, therefore, it may be charge transfer between sulfur and vanadium takes place, but each carbon atom implies four electrons in the outer shell, so carbon atoms trend to consistence covalent bonds, therefore charge exchange may be occur between sulfur atoms and carbon atoms. The bonds which results between carbon and sulfur are not pure covalent and not pure ionic, but it will be partially covalent and ionic bonds. When the interaction between (Ni_4C_4)/(CO_2)$_2$ and sulfur atoms also sulfur atoms trends to make ionic bonds because it have two places in the outer shell may be occupied by the electrons, and the nickel atoms in the organic complex nanostructure trend to make ionic bonds because it has two free electrons in the outer shell, therefore, it may be there are ionic bonds forms between sulfur and nickel, but partially ionic covalent bonds may be form between the sulfur atoms and carbon atoms, hence charge exchange or adsorption procedure may be result between sulfur and carbon. In the interaction between (SiO)$_2$ and each one of the organic complex nanostructures (V_6C_6), (Ni_4C_4)/(CO_2)$_2$, there is covalent bonds may be result between carbon atoms and silicon atoms, so charge transfer or charge exchange may be occur by means of the interaction. Partially ionic covalent bonds may be form between carbon and vanadium or between nickel and carbon.

Electrostatic potentials

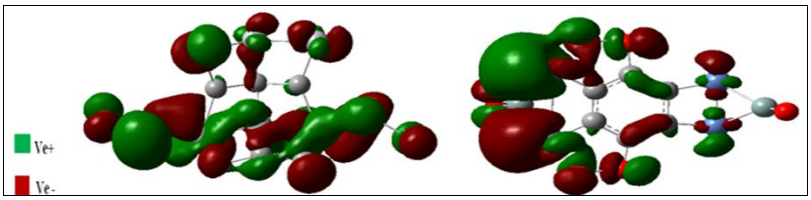
The electrostatic potential characterizes the ability of the molecular system to do work. Each molecular system implies charged particles interact according to the concept of the electrostatic forces. The electrostatic potential occasionally describes by the sum of charges energy. In other sentence it stands for a physics characteristics equal in scalar to the electrostatic energy between point positive charge located at a distance from electronic charges [16]. The electrostatic potential of the nanomaterial structures (V_6C_6), (Ni_4C_4)/(CO_2)$_2$, (V_6C_6)-4S, [(Ni_4C_4)/(CO_2)$_2$]-4S, (V_6C_6)-(SiO)$_2$ and [(Ni_4C_4)/(CO_2)$_2$]-(SiO)$_2$ had been accomplished by employment the density functional theory with sophisticated algorithms in Gaussian 09 program, 6-31G basis set and the hybrid functional B3LYP.



a. (V_6C_6) **b. (Ni_4C_4)/(CO_2)$_2$**



c. (V_6C_6)-4S **d. [(Ni_4C_4)/(CO_2)$_2$]-4S**



e. (V_6C_6)-(SiO)$_2$ **f. [(Ni_4C_4)/(CO_2)$_2$]-(SiO)$_2$**

Fig 2: The electrostatic potential surfaces for the nanostructures (V_6C_6), (Ni_4C_4)/(CO_2)$_2$, (V_6C_6)-4S, [(Ni_4C_4)/(CO_2)$_2$]-4S, (V_6C_6)-(SiO)$_2$ and [(Ni_4C_4)/(CO_2)$_2$]-(SiO)$_2$.

Figure (2) depicts that charge density distribution around most atoms in the organic complex nanostructure (V_6C_6), while in the organic complex nanostructure (Ni_4C_4)/(CO_2)$_2$ the charge density distributes around some atoms more than other atoms. Doping of (V_6C_6) with four sulfur atoms appears the distribution of the electronic charges around the sulfur atoms clearly, one can say the nuclei in the sulfur atoms set a positive test charge near the surface to attract electron of the organic complex nanostructure (V_6C_6) to form ionic bond between vanadium and sulfur, or charge exchange may be happen between sulfur and carbon. The electrostatic potential figure of (V_6C_6)-(SiO)$_2$ depicts charge density distribution concentrates around the two molecules (SiO), hence one can say charge exchange may be takes place between vanadium atoms and silicon atoms or covalent bonds consistence between carbon and silicon or ionic bonds may be consistence between oxygen and vanadium. The electrostatic potential figure of [(Ni_4C_4)/(CO_2)$_2$]-4S demonstrates there is electronic charge distribution about three atoms of sulfur apparently, but there is no electrostatic potential surface around the fourth atom, this occurs because of shielding procedure, in which the atoms in the organic complex nanostructure [(Ni_4C_4)/(CO_2)$_2$]-4S trend to interact with three atoms more than the fourth atom. The shielding procedure happens by means of physical factors just like density of states. One can censor in the interaction between the organic complex nanostructure [(Ni_4C_4)/(CO_2)$_2$] and (SiO)$_2$, the electronic charge distribution about only one molecule SiO, but there is no electrostatic potential surface around the other molecule SiO. One can say the atoms in the organic complex nanostructure [(Ni_4C_4)/(CO_2)$_2$] have a tendency to interact with one SiO molecule, shielding procedure occurs to the other SiO molecule.

Contours

The density of electron charge distribution surrounding the nuclei of atoms has been characterized by contour curves and contour circles maps. Additionally, it express the Fermi level and Fermi energy. The contour maps implies an active locations indicate to the concentration of electronic charges about the nuclei in these locations [17, 18]. There are many physics phenomena, including the charge transfer and charge exchange between the atoms that comprise the geometrical structure may be described by the contour density maps [19]. The contours so express the system's electrostatic potential [20]. The contour density maps of the nanomaterial structures (V_6C_6), (Ni_4C_4)/(CO_2)$_2$, (V_6C_6)-4S, [(Ni_4C_4)/(CO_2)$_2$]-4S, (V_6C_6)-(SiO)$_2$ and [(Ni_4C_4)/(CO_2)$_2$]-(SiO)$_2$ had been achieved by employment the density functional theory with sophisticated algorithms in Gaussian 09 program, 6-31G basis set and the hybrid functional B3LYP.

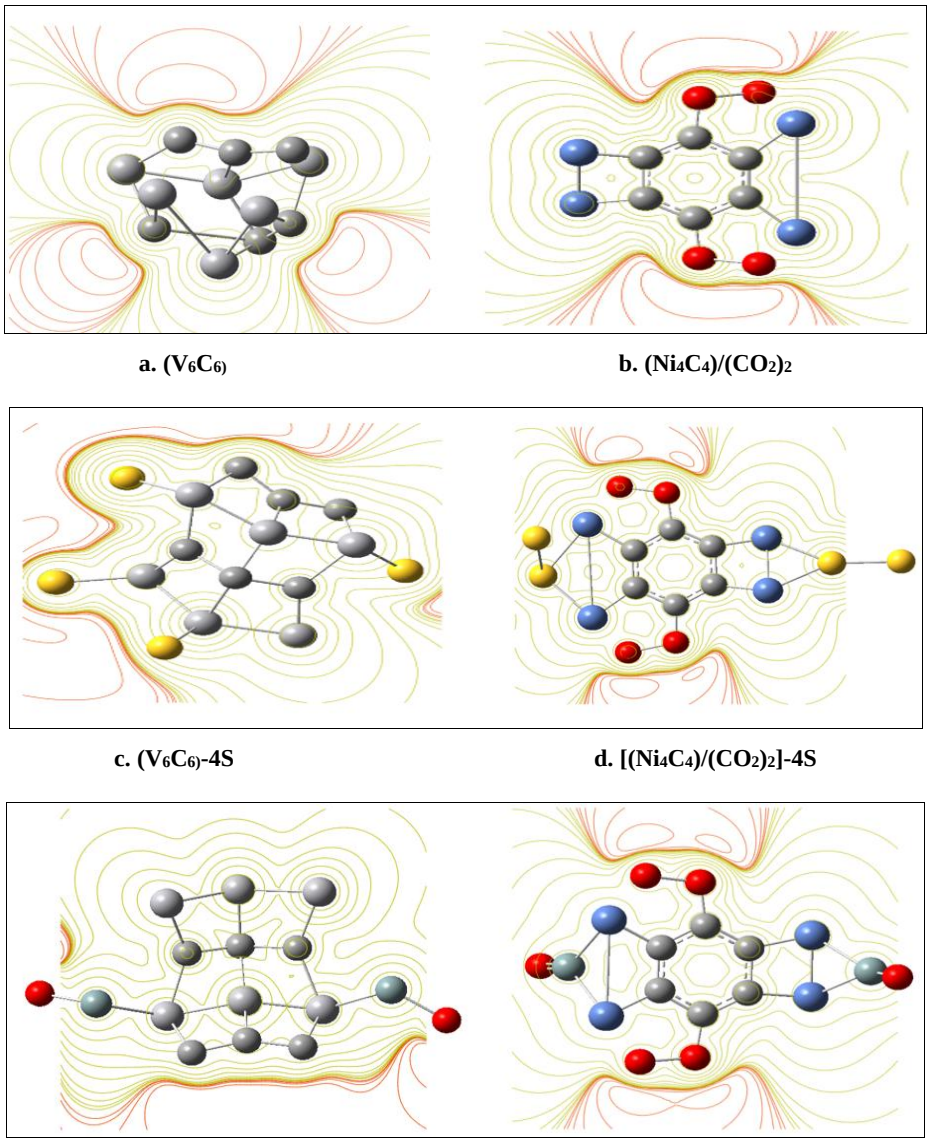
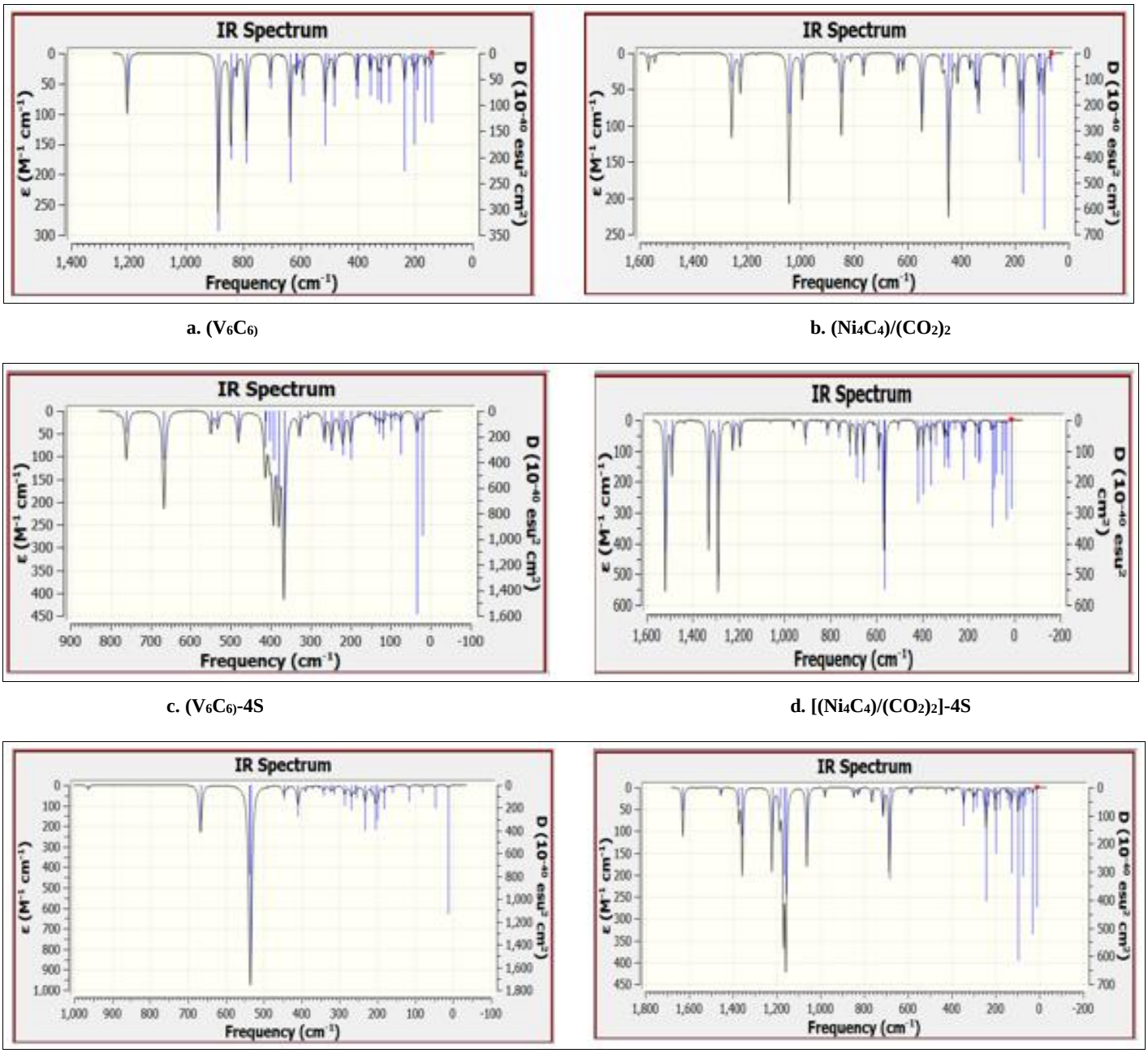


Fig 3: The contour density maps for the nanostructures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$.

In figure (3) one can make a simple rapprochement between (V_6C_6) and (V_6C_6)-4S to see apparent distortion in the contour density maps about the sulfur atoms, and also there is a clear distortion in the density contour maps at the interaction region between sulfur atom with some carbon and vanadium atoms. The distortion in contour maps indicates to the regions of charge exchange and charge transfer. Generally the contour curves or contour circles give an accurate description to the zones of charge transfer or charge exchange. Vanadium atoms implies free electrons in the outer shell, sulfur atoms own two free places in the outer shell, therefore charge transfer may take place from vanadium to sulfur, carbon atoms implies four electrons in the outer shell therefore charge exchange may be occur between carbon and sulfur. A simple comparison between $[(Ni_4C_4)/(CO_2)_2]$ and $[(Ni_4C_4)/(CO_2)_2]$-4S shows contour circles around three sulfur atoms, but there is no contour circles around the fourth atom, hence one can say the charge exchange or charge transfer happen between $[(Ni_4C_4)/(CO_2)_2]$ and three sulfur atoms, while shielding process will take place to the fourth atom by means physics parameters just like the density of states. One can compare between the two interactions (V_6C_6)-4S and $[(Ni_4C_4)/(CO_2)_2]$-4S to watch the distortion in contour maps around sulfur atoms in (V_6C_6)-4S is big as compared with $[(Ni_4C_4)/(CO_2)_2]$-4S. One can see in the interaction (V_6C_6)-$(SiO)_2$, the contour density maps concentrate near some atoms more than other atoms, this signs that the probability of occurring the charge transfer and charge exchange near these positions will be greater. The contour maps express on the Berillon zones, the vacancies between the contour circles stand for forbidden regions, i.e. the electrons cannot exist in this regions.

Infrared spectra (IR)

The infrared schematics characterize the interactions between the substances and the infrared radiation. When the atoms is vibrating atoms and they are of the same type, the symmetric modes are created, but when they are of different sorts, asymmetric modes are created. There are two types of symmetric modes, the first is the elastic and the second is the inelastic [21]. The infrared spectra of the nanomaterial structures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$ had been created by employment the density functional theory with sophisticated algorithms in Gaussian 09 program, 6-31G basis set and the hybrid functional B3LYP.



a. (V_6C_6) **b. $(Ni_4C_4)/(CO_2)_2$**

c. (V_6C_6)-4S **d. $[(Ni_4C_4)/(CO_2)_2]$-4S**

e. (V_6C_6)-$(SiO)_2$ **f. $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$**

Fig 4: The infrared spectra charts for the nanostructures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$.

Figure (4) reveals that the interaction of (sulfur atoms, SiO atoms) with the atoms of organic complex nanostructures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$ tends to appearance of new bonds, the peaks in IR diagrams denotes to the formation bonds. A simple rapprochement between (V_6C_6) and (V_6C_6)-4S shows disappearance some peaks by means of shielding procedure. The peak near the wave number (1200 cm^{-1}) disappears because shielding procedure as a result to the interaction between four sulfur atoms with the organic complex nanostructure (V_6C_6). One can see the peak near the wave number (400 cm^{-1}) was at the intensity (50 M^{-1} cm^{-1}) before the interaction between sulfur atoms and (V_6C_6), but after the interaction between them becomes at (400 M^{-1} cm^{-1}). The increase in the intensity on y-axis happens as a result to the interaction. A simple comparison between $(Ni_4C_4)/(CO_2)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-4S demonstrates new clear peaks next the wave number (1550 cm^{-1}) at the intensity (550 M^{-1} cm^{-1}), also the rapprochement depicts disappearance the peak near (1040 cm^{-1}), this takes place by means of shielding procedure. One can compare between (V_6C_6) and (V_6C_6)-$(SiO)_2$ to observe disappearance most of peaks because of shielding procedure, hence, one can say the atoms in $(SiO)_2$ have a tendency to interact with some atoms in (V_6C_6) more than the other atoms. Comparison between the organic complex nanostructure $(Ni_4C_4)/(CO_2)_2$ and $(SiO)_2$ shows there are new peaks at new wave numbers and new values of intensities point out new bond will originate because of the interactions between $(Ni_4C_4)/(CO_2)_2$ and $(SiO)_2$. The bonds may be Si-C, Si-Ni, SiO, O-O, C-O or Ni-O.

Density of states (DOS)

The number of electronic states within a specific energy domain is determined by the density of states of the electrons in the energy bands. The density of states function is a crucial characteristics in the electronic processes, particularly transport phenomena. So the density of states typifies the

number of electronic states per unit volume in the energy domain. Two basic physics concepts, the Fermi-Dirac statistics and the Pauli exclusion principle are governing the electrons to occupy the energetic levels [22]. The density of states for the nanomaterial structures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$ had been carried out by employment the density functional theory with sophisticated algorithms in Gaussian 09 program with GaussSum03 package.

a. (V_6C_6) ` **b.** $(Ni_4C_4)/(CO_2)_2$

c. (V_6C_6)-4S **d.** $[(Ni_4C_4)/(CO_2)_2]$-4S

e. (V_6C_6)-$(SiO)_2$ **f.** $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$

Fig 5: The density of states plots for the nanostructures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$.

Figure (5) demonstrates influence the interaction between four sulfur atoms and the organic complex nanostructure (V_6C_6) on the density of states. It can be seen that there is new states can be occupied by electrons and also one can see increasing in the number of states at determined values of energy. There was only one state next the value of energy (-18 eV) before the interaction between (V_6C_6) and four sulfur atoms, but after the interaction between them the number of states became three states at the same value of energy. Either one can observe four states can be occupies by electrons next (-7 eV) in the organic complex nanostructure (V_6C_6)-4S, while there were only two states in (V_6C_6). A simle rapprochement between $(Ni_4C_4)/(CO_2)_2$ and $(Ni_4C_4)/(CO_2)_2$-4S demonstrates dissimilarity in the density of states diagram, this means new states refer to new energetic levels can be occupied by electrons as a result to the interaction between sulfur atoms and the organic complex nanostructure $(Ni_4C_4)/(CO_2)_2$. A simple comparison between the organic complex nanostructure (V_6C_6) and (V_6C_6)-$(SiO)_2$ disclosure appearance four states denote to energetic levels can be occupied by electrons next (-5 eV) in (V_6C_6)-$(SiO)_2$ (i.e. after the interaction) as compared with the organic comolex

nanostructure (V_6C_6) (i.e. before the interaction) which has only three states denote to energetic levels can be occupied by electrons. When one make a rapprochement between the organic complex nanostructure $(Ni_4C_4)/(CO_2)_2$ and $(Ni_4C_4)/(CO_2)_2$-$(SiO)_2$ can note four states next the value of energy (-10 eV) before the interaction, but there were only two states after the interaction. Also When one look to the diagrams of density of states can see new states after the interactions near determined values of energy or one may see increasing yin the states next certain value of energy.

Electronic states and energy gaps (Eg)

The energy gap is a physical term that describes the amount of energy needed for an electron to transition from the valence band to the conduction band. According to the physics of solids, the energy needed for an electron to transition from its valence band to its conduction band must be equal to or larger than the band gap. The energy gap is the difference in energy between the lowest vacant orbit energy and the highest occupied orbit energy. Because the valence band and conduction bands are overlap, metallic materials have a zero energy gap. The energy gap is particularly very large in the insulators. The energy gap depends significantly on temperature and impurities. The energy gap value cab be utilized to compare between conductors, semiconductors and insulators. The following is a mathematical expression for the energy gap [23, 24].

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

In terms of HOMO and LUMO energies the energy gap will be

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

Table 1: Illustrates HOMO energies, LUMO energies and energy gaps for the nanostructures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$.

System	E_{LUMO}(eV)	E_{HOMO}(eV)	Energy gap (eV)
(V_6C_6)	-3.0858861	-4.2956427	1.2097566
(V_6C_6)-4S	-4.7081463	-5.8536873	1.145541
(V_6C_6)-$(SiO)_2$	-4.0121145	-5.1179289	1.1058144
$(Ni_4C_4)/(CO_2)_2$	-4.0020468	-4.946778	0.9447312
$(Ni_4C_4)/(CO_2)_2$-4S	-5.292345	-6.2085057	0.9161607
$[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$	-4.9296357	-5.841987	0.9123513

Table (1) demonstrates that the values of energy gaps for all nanostructures trapped between approximately (-0.91 eV) and (1.2 eV), hence, all nanostructures in the table behave as a semiconductors. The energy gap of (V_6C_6)-4S approaches to the energy gap of silicon, (E_g of Si =1.12 eV), this do good in the manufacture of the electronic devices just like the solar cells and photoelectric cells. The energy gap of the nanostructures $(Ni_4C_4)/(CO_2)_2$-4S and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$ closes to the value (0.91 eV), this value be regarded small semiconductor energy gap do good in the photovoltaic systems and transistors. The organic complex nanostructure has energy gap next (1.2 eV), the semiconductors which have energy gap like this be considered advantage in the solar cells and photoelectric cells. The values of HOMO energies and LUMO energies link to tendency of the nanostructures to donate electrons from donor level or accept electrons in acceptor level respectively. The organic complex nanostructure be regarded the best donor among the nanostructures in the table because it has the highest value of HOMO energy, it is (-4.29 eV). The nanostructure $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$ be considered the best acceptor among the nanostructures in the table because it has the minimum value of LUMO energy in the table.

Dipole moment and Polarizabilities

When two charges of the same magnitude but with different signs are separated by a distance r, an electric dipole moment will produce between them if one of them be positive and the other be negative. The Debye unit is named after the physicist, Peter Debye, who was the first to characterize the dipole moment. The electric dipole moments may be induced or permanent. Suppose μ represents the dipole moment, q stands for the charge, and r indicates to the separation between the two charges, the dipole moment can be expressed as [25].

$$\mu = q * r \quad (3)$$

The tendency of molecules to interact with an external electric field produced by another molecule is known as the average polarizability. The equation below provides a mathematical expression for the tensor elements of polarizability, which are based on a second-order derivative of energy in Cartesian coordinates. Suppose the symbols i and j refer to the x and y coordinates respectively. The polarizability will be as folloes [26].

$$\alpha_{i,j} = \frac{\partial^2 E}{\partial F_i \partial F_j} \quad (4)$$

Assume the eigen values of the polarizability tensors are α_{xx}, α_{yy} and α_{zz}, therefore the average polarizability can be calculated from the equation [27].

$$< \alpha > = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (5)$$

Table 2: Exhibits the dipole moment and average polarizability for the nanostructures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$.

System	Dipole moment (Debye)	Average polarizability (a.u)
(V_6C_6)	2.189799	305.756759
(V_6C_6)-4S	8.357457	465.459579
(V_6C_6)-$(SiO)_2$	7.848638	510.260829
$(Ni_4C_4)/(CO_2)_2$	1.353402	245.120663
$(Ni_4C_4)/(CO_2)_2$-4S	2.397810	382.423970
$[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$	1.626828	278.570618

Table (2) demonstrates that the nanostructure (V_6C_6)-4S possesses the highest value of dipole moment in the table, (8.35 Debye). One can note that the sulfur atoms tend to increase the value of dipole moment apparently, it increases

from approximately (2.18 Debye) in (V_6C_6) to approximately (8.35 Debye) in (V_6C_6)-4S. Either one can see that the interaction between the organic complex nanostructure(V_6C_6) and $SiO)_2$ causes increase in the value of dipole moment from approximately (2.18 Debye) in (V_6C_6) to approximately (7.84 Debye) in (V_6C_6)-$(SiO)_2$. The values of dipole moments of the nanostructures (V_6C_6)-4S and (V_6C_6)-$(SiO)_2$ be considered big values make them play an important role in the interactions with the electric fields. All nanostructures in the table have non-zero dipole moment, the lowest value is for the organic complex nanostructure $(Ni_4C_4)/(CO_2)_2$, which equal to approximately (1.35 Debye). The non-zero values because they are hetronuclear structures. The nanostructure (V_6C_6)-$(SiO)_2$ be considered the maximum activity nanostructure by means of it has the maximum value of average polarizability, it is approximately (510.26 a.u). The mateials that have high polarizability has importance in the devices of optics devices, just like the devices which utilize in test the optical characteristics of the substances. Another applications to the high polarizability the communications in the fiber optics.

Symmetry

The mathematical group implies a number of elements that correlate according to a determined rules. The special kind of symmetry that relates to the symmetry of molecular systems is the elements of symmetry. Each one of the symmetry elements there is a symmetry operation. In general, there are seven elements for the symmetry. The seven elements are horizontal axis, identity, dihedral plane, vertical plane, proper axis, improper axis and the inversion center [28, 29]. The symmetry play an active role to know the characteristics of the molecular systems without making computations [30]. The point group symmetries of the nanomaterial structures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$ had been obtained by utilizing the density functional theory with sophisticated algorithms in Gaussian 09 program, 6-31G basis set and the hybrid functional B3LYP.

Table 3: exhibits the point group symmetries for the nanostructures (V_6C_6), $(Ni_4C_4)/(CO_2)_2$, (V_6C_6)-4S, $[(Ni_4C_4)/(CO_2)_2]$-4S, (V_6C_6)-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$.

System	Point group symmetry
(V_6C_6)	C_1
(V_6C_6)-4S	C_1
(V_6C_6)-$(SiO)_2$	C_1
$(Ni_4C_4)/(CO_2)_2$	C_2 / C_1
$(Ni_4C_4)/(CO_2)_2$-4S	C_1
$[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$	C_1

Table (3) demonstrates that the organic complex nanostructure $(Ni_4C_4)/(CO_2)_2$ possesses the point group symmetry (C_2 / C_1). The symbol C_2 in the point group symmetry point out there is two-fold rotational axis of symmetry, this means the organic complex nanostructure will repeat itself after (180º). The interaction between the organic complex nanostructure $(Ni_4C_4)/(CO_2)_2$ with four sulfur atoms, $(SiO)_2$ atoms leads to disappear the point group symmetry C_2, this means the nanostructures after the interactions become repeat itself only after (360º), because it has the type of symmetry C_n, which make the structure repeat itself throughout (360º/n). in the symmetry C_2 (n=2), in symmetry C_1 (n=1). The molecules which implies the point group symmetry (C_2) acquire significance to determine the chirality to develop medicines and designing the cataylists. The molecules which implies the point group symmetry (C_1) acquire importance to understanding the behavior of big biomolecules and the structure of proteins. Another applications to the molecules which has the point group symmetry C_1 are the communications in the networks and quantum cryptography.

Conclusions

Through electrostatic potential pictures, it can be visualized that electronic charges distribution around one of (SiO) molecules but disappear around the other (SiO) molecule when $(SiO)_2$ interact with the organic complex nanostructure $(Ni_4C_4)/(CO_2)_2$, hence one can conclude shielding procedure obtains to one of (SiO) molecules. Depending on the contour density maps one can see in the interaction between (V_6C_6) and $(SiO)_2$, the distortion in contour maps gets at determined regions around some atoms, this confirm the charge exchange at these regions will be stronger than other regions in the molecular structure. The bond at the wave number (400 cm^{-1}) shows shortly corresponding to the intensity (50 M^{-1} cm^{-1}) in the organic complex nanostructure (V_6C_6), but after the interaction with sulfur atoms the same bond demonstrates near the intensity (4000 M^{-1} cm^{-1}). According to schematics of density of states, one can visualize four energetic levels can be occupied by electrons after the interaction between $(Ni_4C_4)/(CO_2)_2$ and $(SiO)_2$ at the energy (-10 eV) instead of two states before the interaction. The nanomaterial structures $[(Ni_4C_4)/(CO_2)_2]$-$(SiO)_2$ and $[(Ni_4C_4)/(CO_2)_2]$-4S have values of energy gap approaches to (0.91 eV), this value of energy gap make them acquire a great significance in the manufacture of photovoltaic systems and transistors. The nanostructure (V_6C_6)- $(SiO)_2$ be considered the highest activity nanostructure among the nanostructures in this paper because it has the maximum value of average polarizability, it approaches to (510.26 a.u). The organic complex nanostructure $(Ni_4C_4)/(CO_2)_2$ has the point group symmetry (C_2 / C_1), The molecules which have the point group symmetry C_2 acquire an importance in the determination of chirality, the development of medicines and designation of cataylists.

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