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The Comparison of Primary, Secondary and Tertiary Amine Ligands on Palladium (II) Complex Ion on Thermo-Physical, Chemical Reactivity, and Biological Properties: A DFT Study

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Abstract. The Palladium is considered as the catalyst for coupling reaction and useful metal in industry. The thermo-physical, chemical reactivity and biological interaction are considered the most expected parameters for use in any area of the chemical industry, the pharmaceutical industry, and academia. The palladium (II) complex ion with different amine ligands are considered under theoretical study by the method of density functional theory (DFT). Some thermo-physical parameters such as free energy, entropy, dipole moment, binding energy, nuclear energy, electronics energy, heat of formation, reactivity properties of molecule like Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO), HOMO-LUMO gap, ionization potential, electronegativity, hardness, softness and electron affinity, and biological properties of molecules like charge density, surface area grid, volume, LogP, polarizibility, refractivity, molecular mass, PIC50 were calculated using the computational program of DFT method. The value of HOMO LUMO gap is 10.78, 0.59, 0.50, and 10.73 and PIC50 is -20.41, -8.46, -1.69, and 1.83 for L01, L02, L03, and L04 respectively while the chemical stability is same for L02, and L03, similarly L01 and L04. The QSAR study provides information about their correlation and biological activity as drugs whereas the biological activity was increased with increasing methyl groups. The four palladium (II) complex ions with amine ligands have strong biological activity for L03 and L04, and occur the correlation on thermophysical, chemical reactivity.

***Keywords*:** Palladium, alkylamine, QSAR, HOMO, LUMO, vibrational spectroscopy and PIC50

Palladium (II) Kompleks İyondaki Primer, Sekonder ve Tersiyer Amin Ligandlarının Termo-Fiziksel, Kimyasal Reaktivite ve Biyolojik Özelliklerle Karşılaştırılması: DFT Çalışması

Özet. Palladyum kenetlenme reaksiyonları için katalizör olarak dikkate alınır ve sanayide kullanışlı bir metaldir. Termo-fiziksel, kimyasal reaktivite ve biyolojik etkileşim, kimya endüstrisi, ilaç endüstrisi ve akademi de en çok dikkate alınan parametrelerdir. Farklı amin ligandları içeren Pd (II) kompleks iyonu, çalışmanın teorik kısmında DFT yöntemi kullanılarak incelenmiştir. Serbest enerji, entropi, dipol moment, bağlanma enerjisi, nükleer enerji, elektronik enerji, oluşum ısısı gibi termo-fiziksel parametreler, HOMO enerjisi, LUMO enerjisi, HOMO-LUMO enerji aralığı, iyonlaşma enerjisi, elektronegatiflik, sertlik, yumuşaklık ve elektron ilgisi gibi reaktivite özellikleri, yük yoğunluğu, yüzey alanı, hacim logP, Polarlanabilirlik, refraktivite, moleküler kütle, PIC50 gibi biyolojik özellikleri DFT methodu yardımıyla hesaplanmıştır. L01, L02, L03 ve L04 için HOMO-LUMO enerji aralığı değerleri 10.78, 0.59, 0.50 ve 10.73; PIC50 değerleri sırasıyla -20.41, -8.46, -1.69 ve 1.83 tür. L02 ile L03 ün, L02 ile L04 ün kimyasal kararlılıkları hemen hemen aynıdır. QSAR çalışması moleküllerin

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biyolojik aktiflikleri hakkında bilgi sağlar. Amin ligandlarını içeren dört Pd(II) kompleks iyonu L03 ve L04 için güçlü biyolojik aktiviteye sahiptir.

***Anahtar Kelimeler*:** Palladyum, alkil amin, QSAR, HOMO, LUMO, titreşim spektroskopisi ve PIC50

1. INTRODUCTION

Palladium is a soft, rare, silvery-white metal that is valued for its catalytic properties and shares many of the characteristics common to the platinum group metal [1]. It has a face-centered cubic crystalline structure at ordinary temperatures and it is strongly resistant to corrosion in the air and to the action of an acid. The largest uses of palladium are as metal in the field of jewelry [2], dentistry, watch making, blood sugar test strips, aircraft spark plugs, surgical instruments, and electrical contacts [3]. On the other hand, these are currently attracted considerable interest because they're potentially beneficial as pharmaceutical ingredients, a bioactive molecule, pharmacological properties [4-6]. Palladium complexes have been worked against cancer cells [7-9]. However, although palladium has less cytotoxic effects than platinum, palladium has good cytotoxic effects as well for use as bioactive molecules of the area drug design [10, 11]. Palladium complexes with aromatic N-containing ligands, e.g., derivatives of amine, pyridine, quinoline, pyrazole, and 1, 10-phenanthroline has shown very promising antitumor characteristics molecules. Some of these complexes, especially the *trans* complexes with non-planar heterocyclic amine ligands have been found to overcome multifactorial *cis* platin resistance in human ovarian cell lines. On the other hand, Pd(II) complexes or complex ions have been widely explored due to their catalytic efficiency, e.g., for various carbon-carbon and carbon-nitrogen bond-forming reactions. The most palladium (0), palladium (II) on carbon makes some versatile catalyst of organic syntheses such as Heck reaction, Suzuki coupling, Tsuji-Trost reactions, Wacker process, Negishi reaction and Stille coupling, etc [12-15]. While most studies of palladium have concentrated on the reactivity of its complexes, little information about their electronic structures has been obtained. Organometallic transition-metal complexes utilizing nitrogen ligands with ionic or polar substituent have been found to catalyze a large variety of chemical transformations in aqueous solution. Palladium is one of the most catalytically versatile transition metal. The nitrogen-containing ligand assisted palladium catalyzed Suzuki coupling reaction is the most frequently employed methods of carbon-carbon bond formation in organic synthesis [14]. In the literature, the molecular structure of a complex containing palladium atom have been studied for years, however electronic structure of this molecule have been worked out quite a bit.

Taking into account all the benefits in thermophysical, chemical reactivity, biological profile, the computational chemistry is the best tools in present time of chemistry, physics, material science, pharmaceutical science, molecular engineering, and biochemistry. To save time and cost, computational computer programming is used on making the correlation of the thermophysical, chemical and biological activity of some palladium complexes. A thermodynamic system is a definite macroscopic area or space in the universe in which one or more thermodynamic processes take place. This system has a specific volume consisting of molecules and atoms with continuous movement and concussion by the interaction with the external surrounding. The internal properties and its interaction with the surrounding determine the system behavior [16-18].

A thermodynamic system can switch from initial state through the intermediate state to the final state which is called transformation of state or thermodynamics process [17, 19]. Using the computational simulation of the examined palladium complexes, It would be calculated by the various method of computational methods. As

the anion has an effective influence on biological activity, the relationship of substituent group in benzene rings was estimated using computing parameters [20, 21]. The most beneficial of the study is the safe the money including conducting a chemical experiment in laboratory and consumption of time in the laboratory at which the most errorless method is the Density functional theory (DFT) [22, 23].

The Density functional theory (DFT) finds an increasingly broad application in the chemical and materials sciences for the interpretation and prediction of complex system behavior at an atomic scale. Specifically, DFT computational methods are applied for the study of systems to synthesis and processing parameters. The Density Functional Theory (DFT) is used to determine chemical structures of molecules and structural changes in molecules. Especially, the B3LYP method is widely used because it yields results very close to experimental results. Moreover, the DFT is a very useful method for predicting the experimental results.

In this study, the palladium (II) complex was synthesized and optimized with DFT/B3LYP. Some geometrical parameters and HOMO-LUMO energy level of the complex were calculated at B3LYP. Their molecular structural relationship, HOMO, LUMO, and quantum chemical properties and LogP plays the role of the chemical reactivity, biological activity and hydrophobicity and hydrophobicity of chemicals in relation with living cells activity and associated mechanistic interactions.

2. COMPUTING METHODS FOR SIMULATION

The molecular modeling program permits to build and analyze different molecular structures and determine the molecular, electronic, and biological properties. In order to create the spatial chemical structure of each calculated molecule, the two-dimensional structure of the molecule shall be built step-by-step by drawing. Then hydrogen atoms are automatically added from building option and chemical structure is converted into a 3D structure. The first step in getting the main characteristic parameters of molecules is to optimize the molecular structure to obtain a configuration characterized by minimum free energy. In sitting the DFT was fixed via 6G-31G*, and B3-LYP [24-26]. After completing optimization, the theoretical properties of the studied compound such as free energy, entropy, dipole moment, binding energy, nuclear energy, electronics energy, the heat of formation, the HOMO, LUMO are recorded. The QSAR properties of molecules like charge density, surface area grid, volume, LogP, polarizability, refractivity, molecular mass, were calculated.

3. RESULTS AND DISCUSSIONS

3.1. Optimized Structure

The symmetry is a very powerful tool to establish the molecular symmetry calculation. In fig-01, Tetraamine palladium (II) complexes ion (L01), Tetra(methylamine) palladium (II) complexes ion (L02), Tetra(dimethylamine) palladium (II) complexes ion (L03) and Tetra(trimethylamine) palladium (II) complexes ion (L04) molecular orbital diagram having both of molecular symmetry and asymmetry properties are represented.

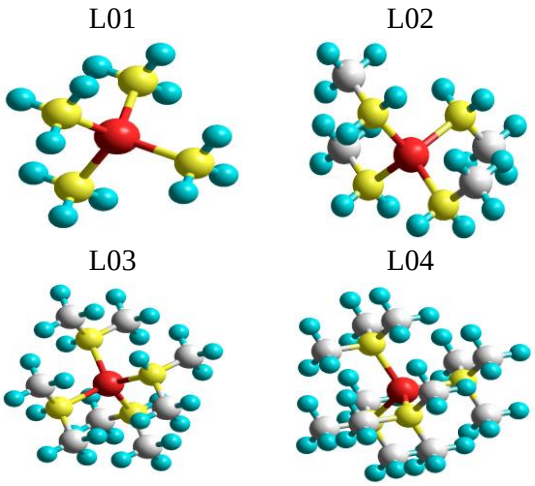


Figure 1. Optimized structure of palladium (II) complex ions with different amine ligands

3.2. Bond Length

In general, the bond length between two atoms is approximately the sum of the covalent radii of the two atoms. For covalent bonds, bond energies and bond lengths depend on many factors like electron affinities, sizes, electronegativity, chemical

reactivity, ionization potential, and chemical stability of atoms involved in the bond. The bond length of atoms in complexes ions are given in fig-02. The bond length in palladium (II) with nitrogen is 2.03 for all complexes.

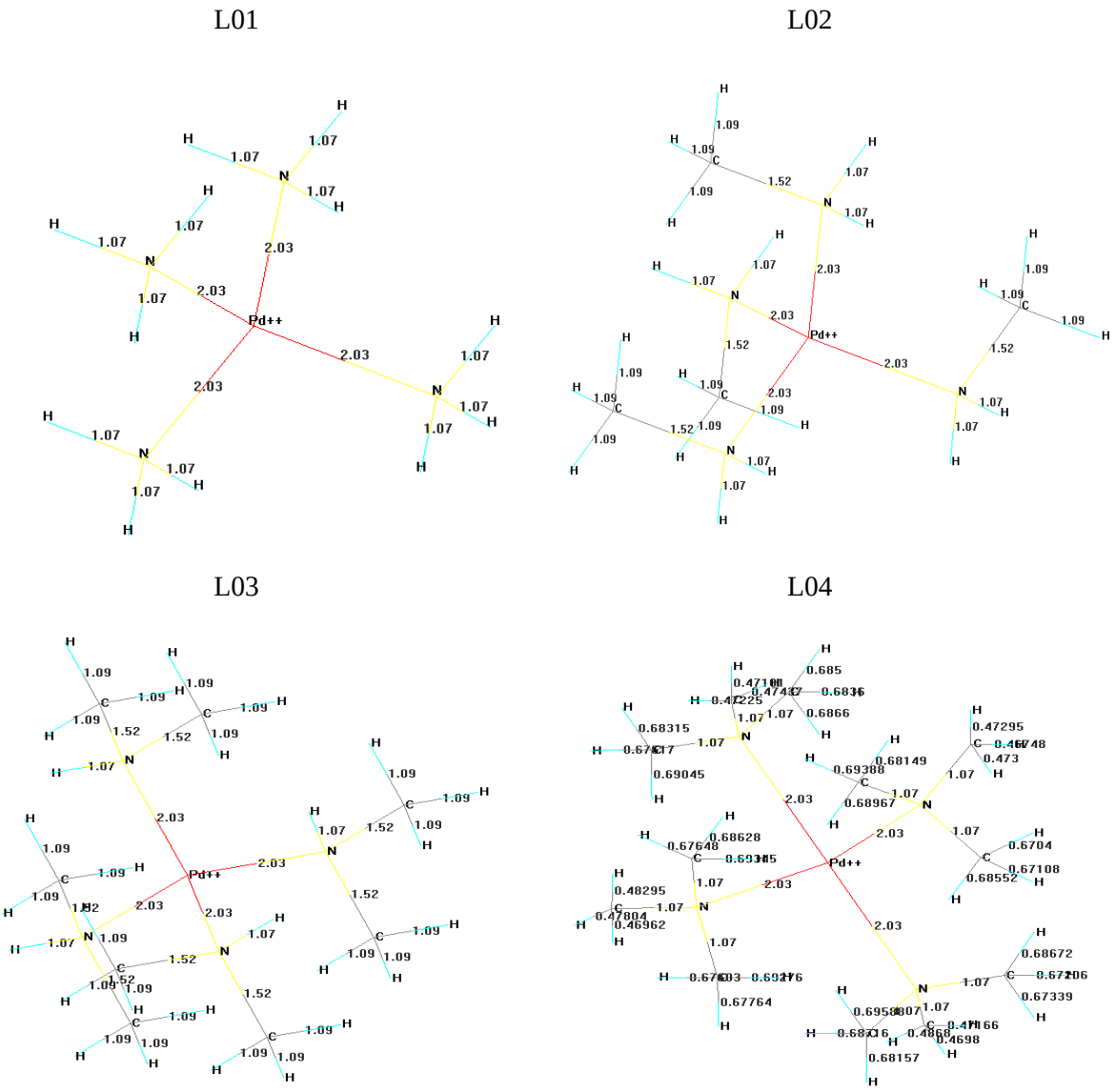


Figure 2. Bond length of palladium (II) complex ions with different amine ligands

3.3. Bond Order

The bond order indicates the chemical stability. The higher the bond order indicates the stronger the pull between the two atoms and the shorter the bond length. The shorter bond length indicates the higher required energy, as a result, the rate of reaction decreases and chemical reactivity decreases [27]. From figure 03, the bond order between all atoms in a molecule is obtained in same and that is one.

3.4. The Atomic Charges

The atomic charge is the most important parameters for calculation of thermophysical properties and thermodynamics shown in fig 4. In L01, the atomic charge of palladium atom is 1.057, and a nitrogen atom in amine ligands almost 0.300 to 0.397 and carbon atom in the methyl group is 3.96 to 3.99.

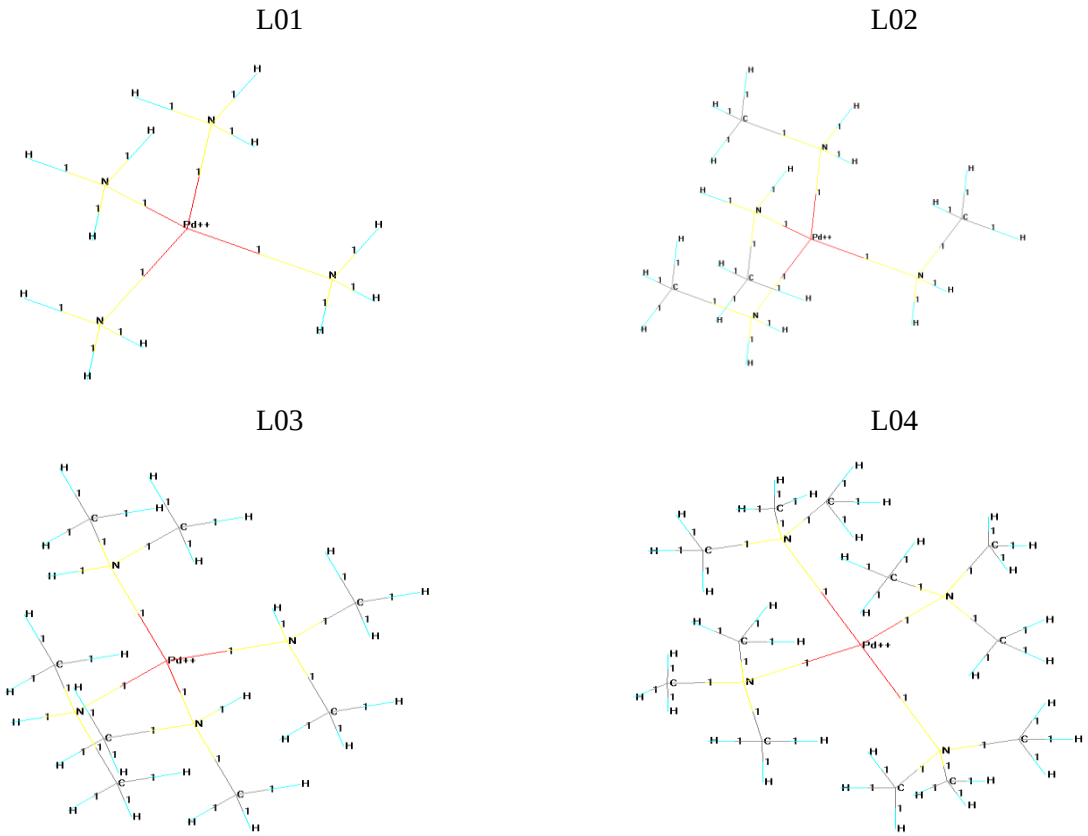


Figure 3. Bond order of palladium (II) complex ions with different amine ligands

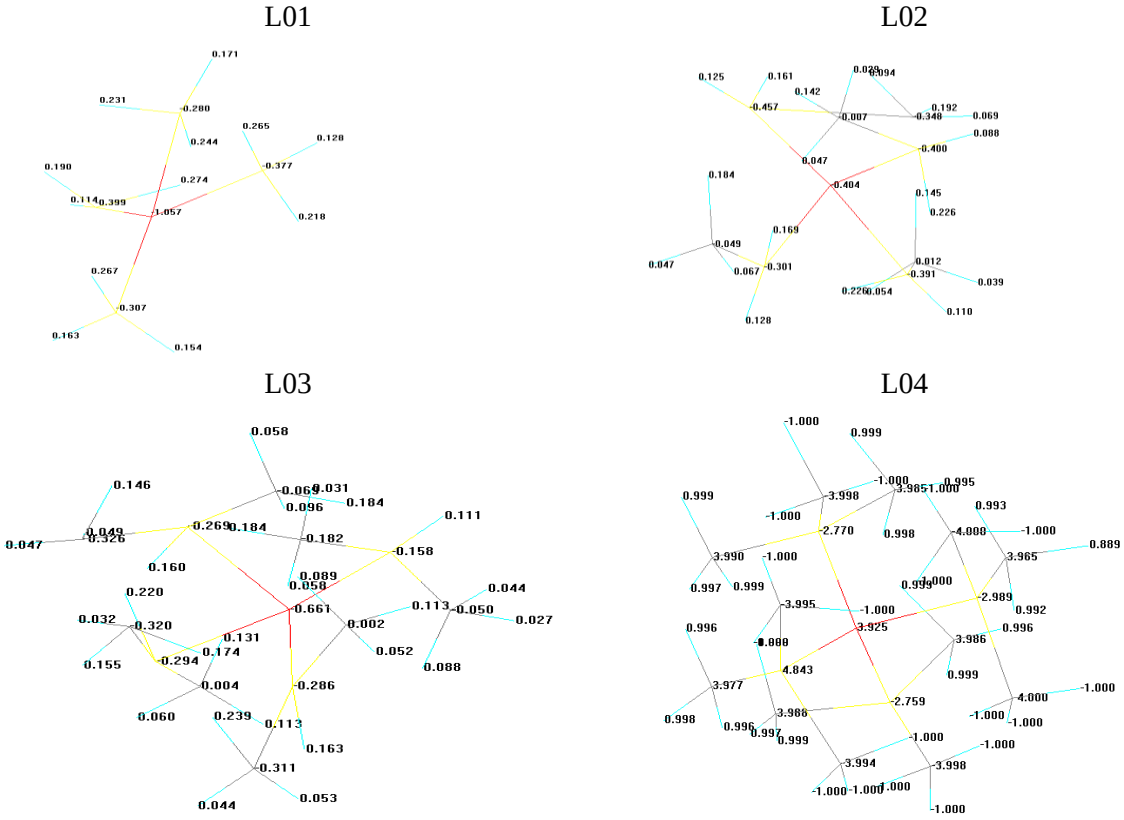


Figure 4. Atomic charge of palladium (II) complex ions with different amine ligands

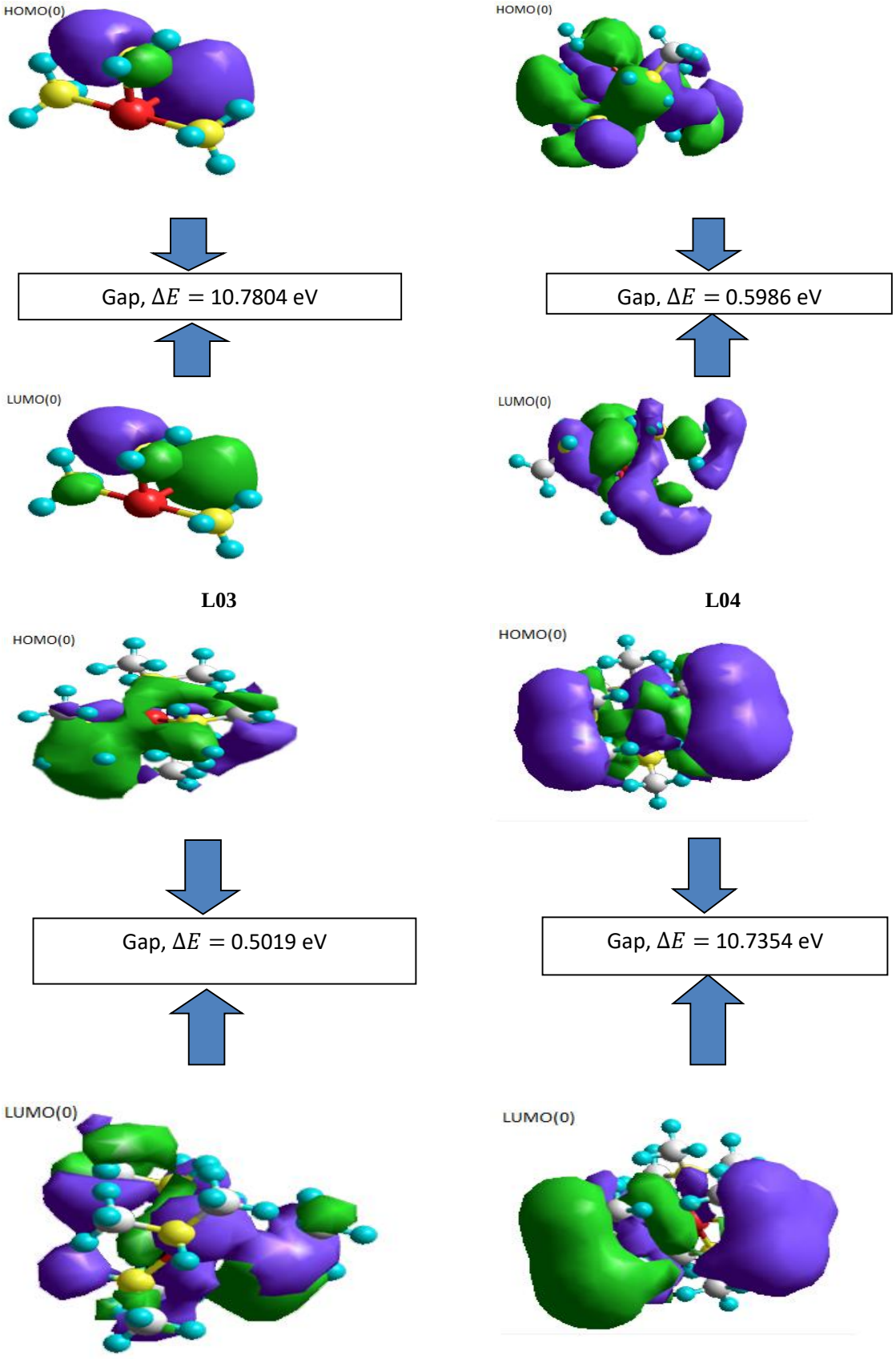


Figure 5: Orbital picture of HOMO and LUMO palladium (II) complex ions with different amine ligands

3.5. HOMO-LUMO

The energy levels of the molecular orbitals order HOMO and LUMO for palladium (II) complexes ion with different amine ligands give information on the possible electronic transition and chemical stability. The HOMO and LUMO also indicate the electrophilic and nucleophilic attraction region in the molecule. The LUMO-HOMO gap is the most important parameter for chemical reactivity [28]. The shorter LUMO- HOMO gap is considered as the high reactivity, they are highlighted in figure 5 (color: green is a positive value and blue is a negative value). The HOMO can be through the outermost orbital containing electrons tends to give these electrons such as an electron donor. On the other hand, LUMO can be through the innermost orbital containing free places to accept an electron.

Table 1. Data for HOMO LUMO in different transition state

	L01	L02	L03	L04
HOMO(0), eV	-16.1487	-18.05713	-23.64721	-37.68882
HOMO(-1), eV	-5.360071	-17.45854	-23.14531	-26.95374
HOMO(-2), eV	-4.970126	-17.22483	-21.69175	-19.8055
LUMO, (0), eV	-5.360071	-17.45854	-23.14531	-26.95374
LUMO, (-1), eV	-16.1487	-18.05713	-23.64721	-37.68882
LUMO, (-2), eV	-17.39359	-18.3907	-23.9424	-37.84376

3.6. Chemical reactivity by DFT Calculations

The Energy of the HOMO is directly related to the ionization potential and LUMO Energy is directly related to the electron affinity. The energy difference between HOMO and LUMO orbital is called an energy gap which is an important parameter that determines the stability of the structures. The energy gap is used in determining molecular electrical transport properties. In addition, according to Koopmans' theorem the energy gap, Egap, defined as the difference between HOMO and LUMO energy [29].

$$\mathrm{E_{gap}} = (\mathrm{E_{LUMO}} - \mathrm{E_{HOMO}}) \approx \mathrm{IP} - \mathrm{EA}$$

The ionization potential (I) and electron affinity (A) can be estimated from the HOMO and LUMO energy values as following

$$I = -E_{HOMO} \quad (1)$$

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

Table 2: Data for HOMO, LUMO, IP, EA, and LUMO- HOMO gap, (ΔE)

	L01	L02	L03	L04
HOMO, eV	-16.1487	-18.0571	-23.6472	-37.6888
LUMO, eV	-5.3601	-17.4585	-23.1453	-26.9534
ΔE, (LUMO-HOMO gap), eV	10.7804	0.5986	0.5019	10.7354
Ionization potential (I),eV	16.1487	18.0571	23.6472	37.6888
Electron affinity (A),eV	5.3601	17.4585	23.1453	26.9534

3.7. Chemical reactivity by DFT Calculations

Entropy and enthalpy is an important part of thermodynamics, which allows physics and physical chemistry to participate in any system throughout physical and chemical change. Entropy and enthalpy are closely related to each other. Entropy can be understood as the discharge condition of any substance, i.e., whose entropy value is greater than its distortion in the reaction

of the participant. Table 3 shows that at the zero temperature without electric field, the value of

entropy of optimized molecule is zero. On the other hand, it is found from table 4 that entropy and heat of capacity is increased with increasing temperature.

Table 3: Thermophysical properties

Properties	L01	L02	L03	L04
Total energy, (kcal/mol)	-3159536.19	-3273037.55	-3311028.49	-3015629.47
Entropy, (kcal/mol-deg)	0	0	0	0
Free energy, (kcal/mol)	-3159536.19	-3273037.55	-3311028.49	-3015629.47
Heat capacity, (kcal/mol-deg)	0	0	0	0
Dipole moment, (D)	0	0	0	0
RMS gradient, (kcal/mol)	0	0	0	0
Binding energy, (kcal/mol)	-3159536.19	-3273037.55	-3311028.49	-3015629.47
Electronic energy,(kcal/mol)	-3580683.64	-3976688.55	-4438431.58	-4654099.65
Nuclear energy, (kcal/mol)	421147.450	703650.999	1127403.091	1638470.185

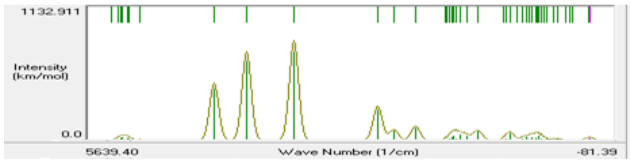
Table 4: Entropy and Heat capacity in different temperature

	273 K		298 K		323 K	
	Entropy	Heat capacity, (kcal/mol-deg)	Entropy	Heat capacity, (kcal/mol-deg)	Entropy	Heat capacity, (kcal/mol-deg))
L01	0.07008	0.010338	0.0712	0.0107	0.0722	0.0112
L02	0.07046	0.007458	0.0713	0.0077	0.0721	0.0080
L03	0.07200	0.007138	0.0729	0.0074	0.0737	0.0077
L04	0.07498	0.008278	0.0758	0.0085	0.0768	0.0088

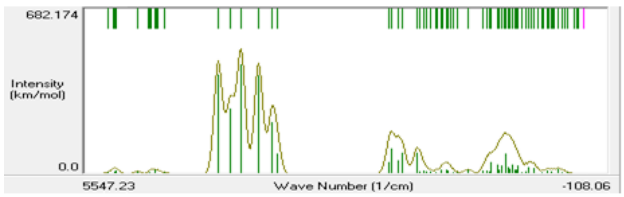
3.8. Vibrational spectrum

The vibrational spectrum is the characteristic peak of any molecule for identification similar to the FTIR peak. To optimize these molecules for vibrational peak obtain the identified peak in the different region about 0 to 5800 cm^{-1} at which the main characteristic peak of tetraamine palladium(II) complex ion is almost 4200-4300, 3825- 3900 and 3600-3550 cm^{-1} and represented in fig-06.

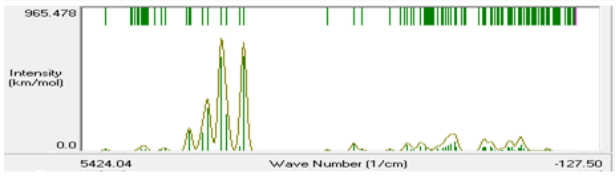
L 01



L 02



L 03



L 04

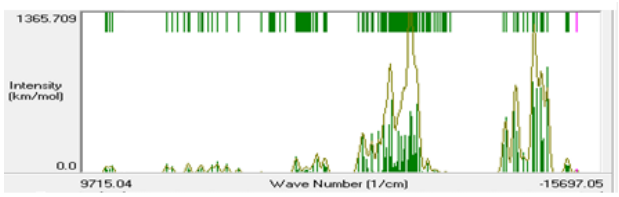


Figure 6. Vibrational spectrum

Table 5. Data for a vibrational spectrum of palladium (II) complex ions

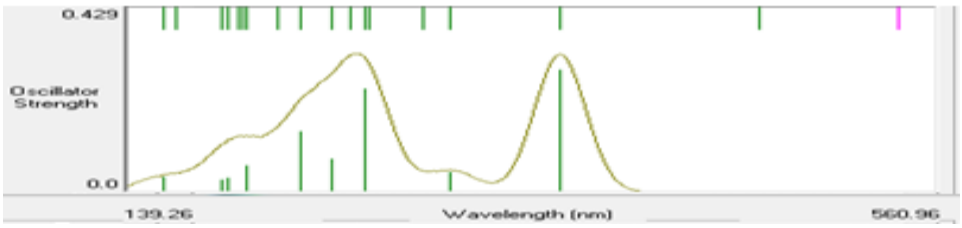
	Normal mode	Degeneracy	Frequency	Intensity	Symmetry
L01	1	1	178.65	18.201	1 A
L02	1	1	149.0	0.994	1 A
L03	1	1	124.84	0.517	1 A
L04	1	1	-14541.96	37.383	1 A

3.9. UV-visible Spectrum

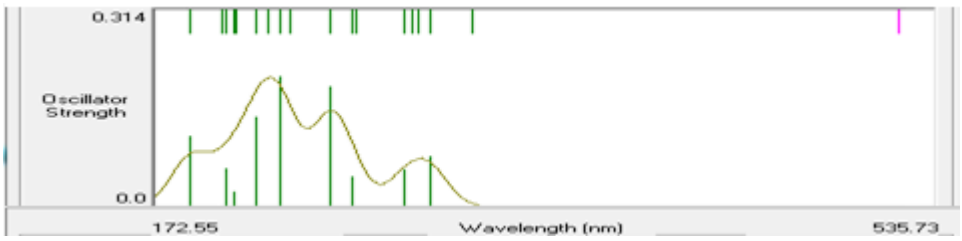
UV-visible Spectrum provides a powerful technique by which the nature of metal ligands bonding may be identified. A remarkable covalency between almost all of the upper filled molecular orbitals of the ligand cluster and the metal d orbitals of suitable symmetry can be calculated. Those interactions which arise from ligand orbitals of n symmetry primarily involve filled metal 4dxz and 4dyz orbitals and, although of importance, do not result in significant Pd (II) overlap since contributions due to filled bonding and anti-bonding levels tend to cancel one another. However, the interactions with orbitals of symmetry involve empty 4dxy and 5s metal orbitals and result in important ligand-to-metal charge transfer [30].

The UV-visible spectrum of the tetra-amine palladium (II) complex ion shows in fig 7 with table 6, a strong transition (e near 250 and 360 nm, as well as an ultraviolet band of weaker intensity near 320 nm.

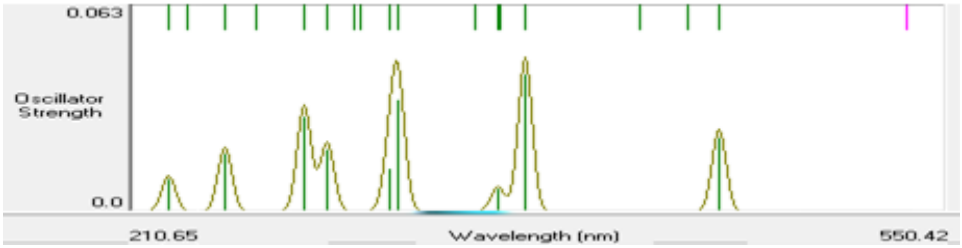
L01



L02



L03



L04

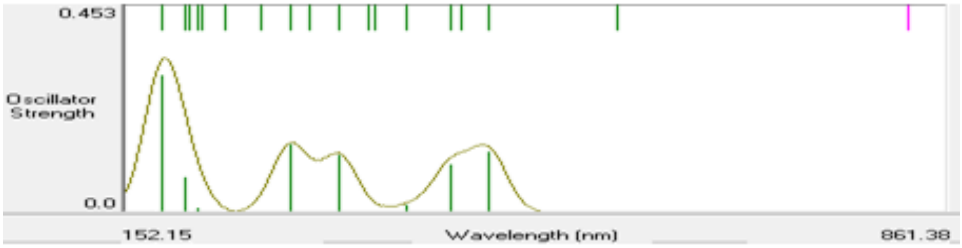


Figure 7: UV-visible Spectrum

Table 6. Data for different transition state, spin multiplicity, wavelength and oscillator strength for UV –visible spectrum

	Transition	Degeneracy	Spin Multiplicity	Wavelength	Oscillator Strength
L01	1	1	Triplet	541.79	0.0
L02	1	1	Triplet	519.22	0.0
L03	1	1	Triplet	534.98	0.0
L04	1	1	Triplet	829.14	0.0

4. THE BIOLOGICAL ACTIVITY OF OPTIMIZED MOLECULES

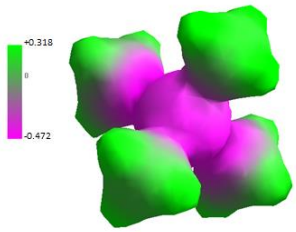
4.1. The distribution electrostatic potential in case of 3D mapped structure

The stability of the studied molecular structure is given by the higher negative values of total energy. The biological activity of a compound can be estimated on the basis of the energy difference ΔE frontier orbitals given in table-07. This difference, ΔE represents the electronic excitation energy which is possible in a molecule. The electrostatic potential in view of the 3D mapped structure in fig 08 indicates positive and negative charge region and the charged surface area in a molecule that is considered as the best tools to estimate the biological activity parameter [31].

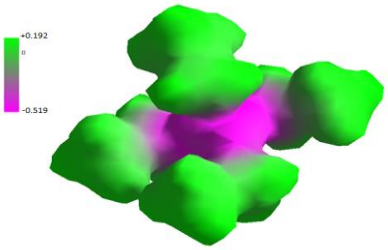
According to the mechanism of antimicrobial activity and antimicrobial agents of bioactive molecules, the positive charge end of molecules is responsible to damage the plasma membrane of pathogens [32]. To kill the different human pathogenic microorganism, the region of molecules was used the positive charge area of the molecule. In this case, the most important factors are explained that the higher surface area having a positive charge is considered as the high antimicrobial activity.

The three-dimensional geometry of molecular electrostatic potential distribution highlights the existence of three regions with increased electronegativity in the whole molecule of L01, L02 and highly positivity in L03 and L04 shown in fig-08 and which play a role in their coupling to different structures in which ions are positively charged.

L01



L02



L03 L04

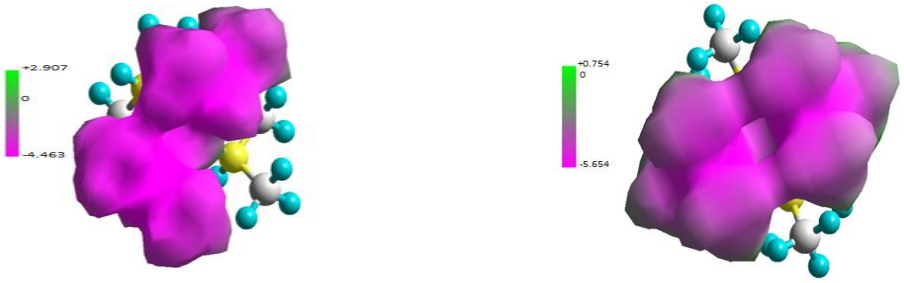


Figure 8: The 3D geometry of the distribution electrostatic potential

Table 7. Data of electrostatic potential energy difference of two levels

	L01	L02	L03	L04
E1	+0.318	+0.192	+2.907	+0.754
E2	-0.472	-0.519	-4.463	-5.654
ΔE= E2-E1	-0.790	-0.711	-7.370	-6.408

Here, E1 = Electrostatic potential energy in positive value, E2 = Electrostatic potential energy in negative value and ΔE = Electrostatic potential energy difference of two level.

4.2. Chemical reactivity

The HOMO and LUMO energies are used for the determination of global reactivity descriptors. It is important that electrophilicity (ω), the chemical potential (μ), electronegativity (χ), hardness (η) and softness (S) be put into a molecular orbital's framework. We focus on the HOMO and LUMO energies in order to determine the interesting molecular/atomic properties and chemical quantities. These are calculated as following equations, and given in table 08.

$$(\mu) = -\frac{I+A}{2} \quad (3)$$

$$(\eta) = \frac{I-A}{2} \quad (4)$$

$$(S) = \frac{1}{\eta} \quad (5)$$

$$(\chi) = \frac{I+A}{2} \quad (6)$$

$$(\omega) = \frac{\mu^2}{2\eta} \quad (7)$$

Table 8. Chemical reactivity

	L01	L02	L03	L04
Hardness, (η)	5.3943	0.2993	0.2509	5.3677
Softness, (S)	0.1854	3.3411	3.9856	0.1863
Electrophilicity (ω),	10.7203	526.7949	1090.8466	97.3092
Chemical potential, (μ)	-10.7544	-17.7578	-23.3963	-32.3211
Electronegativity, (χ)	10.7544	17.7578	23.3963	32.3211

4.3. Quantitative structure - activity relationships (QSAR)

The molecule with minimum binding energy will have the maximum binding affinity and having the maximum binding affinity, indicating as the best molecule for drug leads molecules targeting computationally. In case of the biological activity of a molecule, the surface area is considered as an important parameter. Greater charge surface area of a molecule can be able to kill more pathogens. The greater positive charge surface area means a higher biological activity. On the other hand, a negative value of logP indicates the hydrophilicity and positive LogP indicates the hydrophobicity that plays an important role in biochemical interactions and bioactivity [33, 34].

Hydrophobic drugs tend to be more toxic because, in general, are kept

longer, have a wider distribution in the body, are somewhat less selective in their binding to molecules and finally are often extensively metabolized.

Finally, the correlation of L01, L02, L03, and L04 complexes ion are increased the biological activity as increasing the size of ligands with fine correlation showing in table 09.

4.4. Calculation of PIC50

The correlation between the biological activity and descriptor is developed by Zineb Almi et.al. 2014 [35] for the PIC50 value calculation from the Hyperchem simulation value that is given in the following equation as:

$$PIC50 = 3.028 - 0.542\log P + 0.352\,HE - 1.272\,Pol + 0.863MR - 0.038\,MV - 0.024MW + 19.120q01 + 0.024SAG$$

Here, HE = Hydration Energy, Pol = Polazibility, MR = Molecular Refractivity, LogP = Partition coefficient, MV = Molar Volume, MW = Molar Weight, SAG = Surface Area Grid, q01 = atomic net charges.

According to Zineb Almi et.al. 2014 [35], the biologically active molecule have PIC50 less value -200. From the table 10, the computed molecule of palladium (II) complex ion has the value of more 20 to 225 that means have biological activity and increasing length or number of methyl groups in amine ligands, the biological activity increases. In the L03 and L04 have the highest biological activity near to standard bioactive molecules.

Table 9. Data for QSAR study

	L01	L02	L03	L04
Partial charge (e)	0.00	0.00	0.00	0.00
Surface Area(grid),	286.86	365.65	412.23	439.46
Volume, $Å^3$	401.50	586.90	713.83	806.95
Hydration Energy kcal/mol	-43.34	-10.91	0.86	4.79
Log P	-3.91	-2.93	-1.94	-0.95
Refractivity $Å^3$	9.60	29.19	48.77	68.36
Polarizibility, $Å^3$	4.74	12.08	19.42	26.76
Mass (amu)	174.52	230.63	286.74	342.84

Table 10. Data of PIC50

	L01	L02	L03	L04
PIC50	-20.41	-8.46	-1.69	1.83

4.5. Correlation and comparison study in case of substituent groups in amine ligands

In the case of chemical reactivity, the LUMO-HOMO gap in presence of H atom in NH_3 and $3CH_3$ in N-atom is 10.7804 and 10.7354 eV which is larger value meaning lower reactivity and almost the same. On the other hand, attaching one and two methyl group in amine ligand, the LUMO-HOMO gap is 0.5986 and 0.5019 eV which means that attaching two methyl groups has higher reactivity that one methyl group.

The most important comparison in thermophysical properties is explained that with increasing the temperature, the entropy and heat capacity increases in poor amount and with increasing methyl group in amine ligand the entropy change is an amount of 0.00 0.00038, 0.00154 and 0.0029 kcal/mol. The heat capacity

is also decreased as $3CH_3 < 2CH_3 < CH_3 < H$ or
primary < secondary < tertiary.

Table 11: Correlation among all palladium (II) complex ions

	Pi, π		Refractivity, (MR)		Surface Area, (SA)	
Pi, π		Biological activity		Biological activity	SA	Biological activity
H	0.0	--	0.0	--	0.0	Correlation occurs
CH_3	-0.98	Less	+19.59	Less	+78.79	
$2CH_3$	-1.97	Less	+39.17	Less	+125.37	
$3CH_3$	-2.96	Less	+58.76	Less	+152.60	

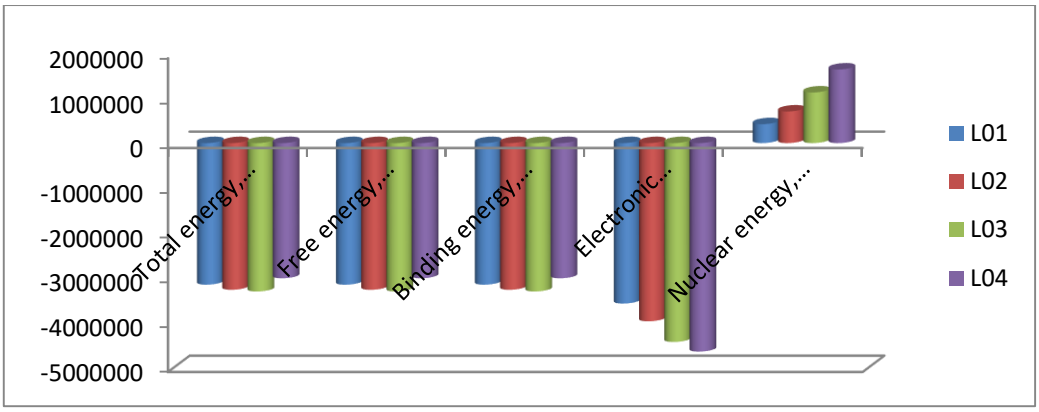


Figure 9. Comparison of thermophysical properties

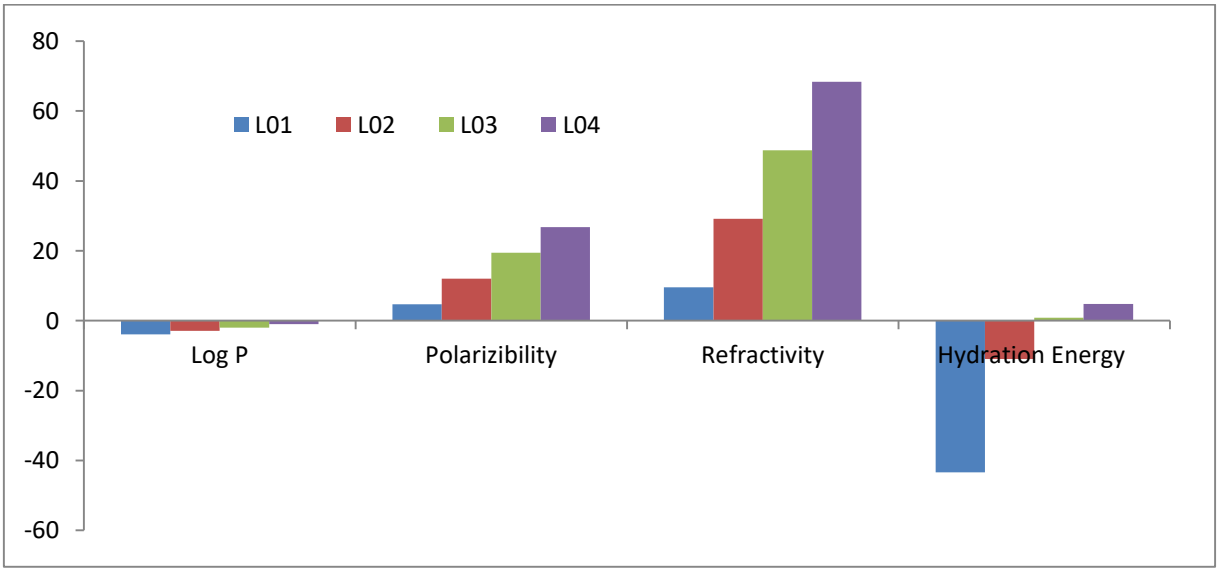


Figure 10. Comparison of QSAR

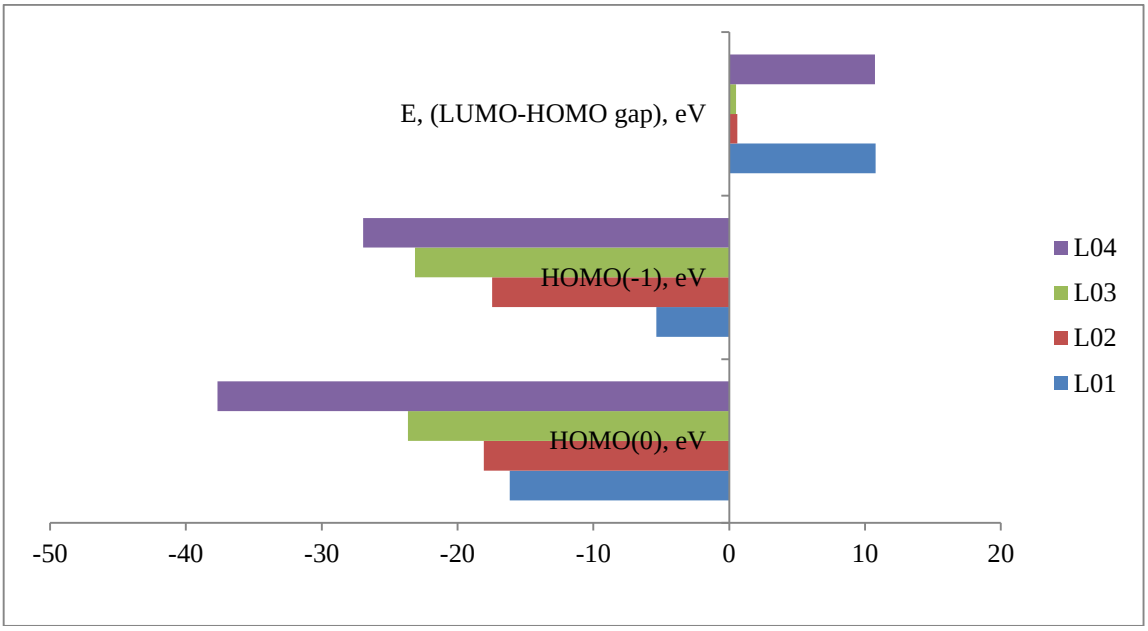


Figure 11. Comparison of the gap with chemical reactivity

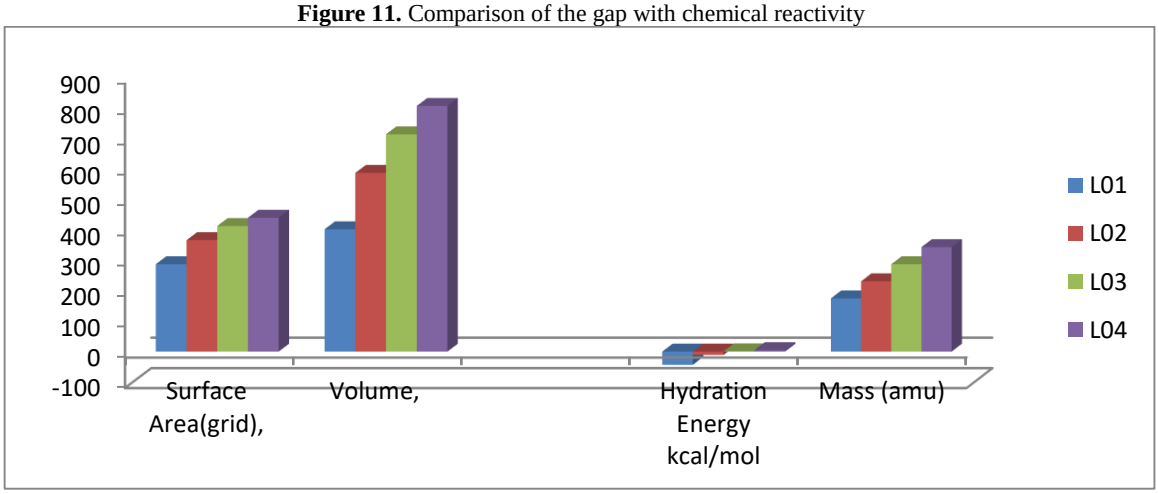


Figure12. Comparison of molecular properties

From figure 9, 10, 11, 12, it was found that biological activity increases with the increase the alkyl groups in palladium (II) complex ions.

5. CONCLUSION

The DFT method was used to characterize and optimize of palladium (II) complex ions with amine ligands and the thermophysical and chemical and biological properties were recorded. From the spectroscopy studies, the vibration, degeneracy, symmetry, and splitting of d orbitals give the information in the analytical method. In the case of HOMO, LUMO, and HOMO – LUMO gap can be informed that palladium (II) complex ions with amine ligands are chemically reactive for further uses. As the value of LogP is negative, palladium (II) complex ions with amine ligands are hydrophilic nature that is why the toxicity is very less and supports the safe uses in all areas.

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