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Original Article

The Evaluation and Comparison of Thermo-Physical, Chemical and Biological Properties of Palladium(II) Complexes on Binuclear Amine Ligands with Different Anions by DFT Study

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ABSTRACT

As cancer is the top killer diseases in the world, the scientists and researchers have been searching the new drugs and remedy methods. Most of the anticancer drugs are organic compounds which were approved by the FDA while metallodrugs are very rare. In the present time, some palladium and rhodium complexes are going to use as anticancer molecules. The palladium(II) complex has higher anticancer activity against different cancer cell that is why the different amine ligands are considered under theoretical study by the method of density functional theory (DFT) to make a new molecule. Some thermo-physical parameter was conducted such as free energy, entropy, dipole moment, binding energy, nuclear energy, electronics energy, the heat of formation. On the other hand, the chemical reactivity properties 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 like charge density, surface area grid, volume, LogP, polarizability, refractivity, molecular mass were calculated using the DFT method. To make comparative biological properties, different anions such as chloride, nitrate, hydroxide, carbonate and sulfate ions were used as homogeneous and heterogeneous adding.

Key words: Palladium(II), QSAR, HOMO, LUMO, Vibrational spectroscopy and Electronic spectroscopy.

Introduction

During the present time, the cancer diseases are growing at alarming rate which is already considered as threatening for human and the best-killing agents worldwide. In

this case, there is an essential need for the development and screening of potential anticancer agents. Most of anticancer agents and therapy were related to organic molecules and not highly effective. During the last five years, some organometallic complexes were used as anticancer drugs. Among them, the palladium, platinum, bismuth and rhodium complexes are using to make new anticancer agents against a wide majority of cancer type, and are the most widely known metal-based anticancer drug. Palladium-based new therapeutic agent was found to be used for the application of transition metal complexes for therapeutic design.

The palladium is also known as the versatile catalyst for coupling reaction in organic chemistry and useful metal in the chemical industry (Chen *et al.,* 2009). The palladium(II) complex has low cytotoxicity (Lazarević *et al.*, 2017) and anticancer properties against different cancer cell (Ray *et al.*, 2007). To estimate the biological activity of palladium(II) complex, some computing method from computational chemistry overviews was performed for calculating different properties. 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 (Kumer *et al.*, 2019a; Kumer *et al.*, 2019b).

Since the more prevalent application of density functional theory (DFT) calculations in the field of chemistry, material science, and drug design in the last 30 years, organometallics and computational chemistry have to be converted into a nondissociable pair. Due to gain the Nobel Prize awarded in 2010 to Heck, Negishi, and Suzuki for Palladium-catalyzed cross-coupling reactions for the widely used class of transformation of organic synthesis, the experimental work was being a lot in the last 10 years (Miyaura and Suzuki, 1995; Miyaura *et al.,* 1981). But there have been quite a few evolutions and works which will try to describe the main theoretical data and study. In recent time, some physical and thermophysical, reaction mechanism and chemical kinetics research were been being and in views of DFT which is not enough to predict and design the new bioactive molecules and their biological properties that is why in this work, is focused on concepts and theoretical study on thermophysical, thermochemical, chemical reactivity and biological activity (Hossain and Kumer, 2018; Kumer *et al.,* 2017).

Palladium(II) complexes currently attract considerable interest because of their potentially beneficial pharmacological properties (Doucet and Hierso 2007; Garrett and Prasad, 2004). Palladium complexes have been worked against cancer cells. However, although palladium has less cytotoxic effects than platinum, palladium has good cytotoxic effects as well. In this study, the palladium(II) complex was optimized with DFT/B3LYP. Some geometrical parameters, HOMO, LUMO, HOMO-LUMO gap and LogP play the role of the chemical reactivity, biological activity. The LogP predicts the hydrophilicity or hydrophobicity of molecule which is considered as the parameters of toxicity. The HOMO and LUMO energy level of the complex was calculated at B3LYP of DFT. On the other hand, the QSAR study provides the statistical data of biological and pharmacokinetics by which these molecules are considered as a new drug or bioactive molecule.

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 (Koopmans, 1934).

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

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

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

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

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 properties and chemical quantities are calculated as the following equation

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

$$(\eta) = \frac{I-A}{2} \quad (5)$$

$$(S) = \frac{1}{\eta} \quad (6)$$

$$(\chi) = \frac{I+A}{2} \quad (7)$$

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

To design the new bioactive molecules, the binuclear ligands were used which is attached with the palladium(II) ion to form different palladium(II) complexes with binuclear ligands. In this case, the hydrazine is selected as a primary ligand and increasing one carbon atom in the next compound. Similar way, the hydrazine, ligands were used to make a comparative activity study on basis of alkyl chain for biological study.

Materials and methods

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

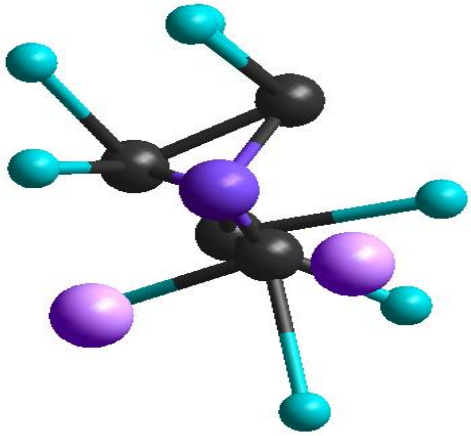
characterized by minimum free energy. In sitting the DFT was fixed via 6G-31G*, and B3-LYP (Howard *et al.,* 1994). After completing optimization, the theoretical properties of the studied compound such as free energy, entropy, dipole moment, binding energy, nuclear energy, electronics energy, the heat 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. Using the computing in vibrational optimization, the UV-visible spectroscopy and IR spectroscopy were determined.

Results and discussions

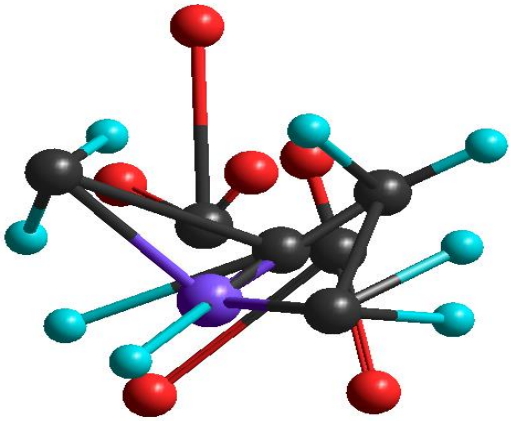
Optimized structures

The symmetry is a very powerful tool to establish the molecular symmetry calculation. In fig-01, the palladium(II) complex like L01, L02, L03, L05, L06, L07, and L08 are presented of a molecular orbital diagram having both of molecular symmetry and asymmetry properties.

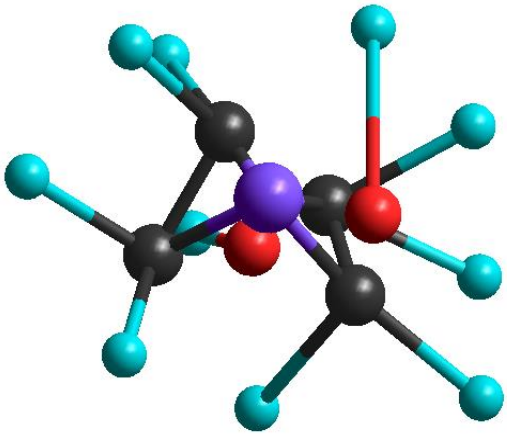
Dihydrazine palladium(II) chloride (L01)



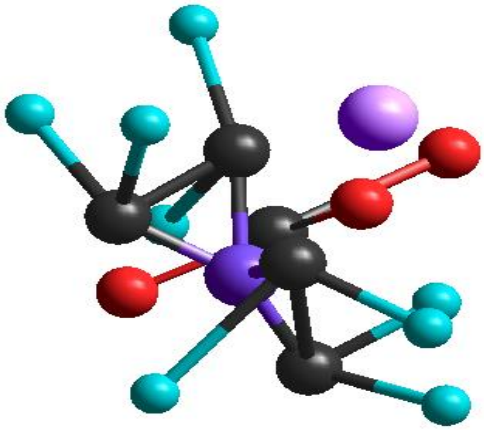
Dihydrazine palladium(II) nitrate (L02)



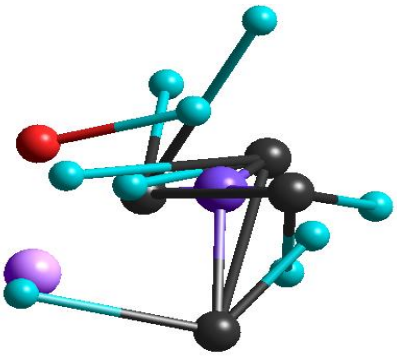
Dihydrazine palladium(II) hydroxide (L03)



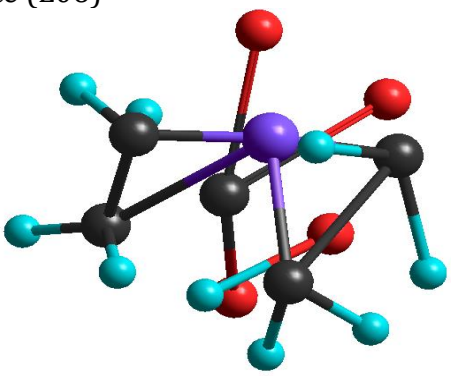
Dihydrazine palladium(II) chloride nitrate (L04)



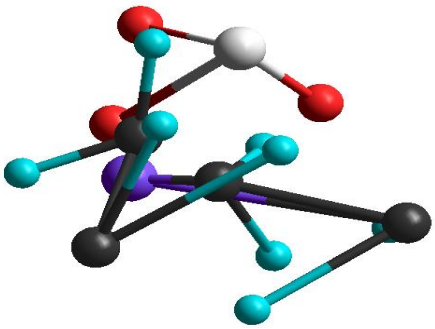
Dihydrazine palladium(II) chloride hydroxide (L05)



Dihydrazine palladium(II) hydroxide nitrate (L06)



Dihydrazine palladium(II) carbonate (L07)



Dihydrazine palladium(II) sulfate (L08)

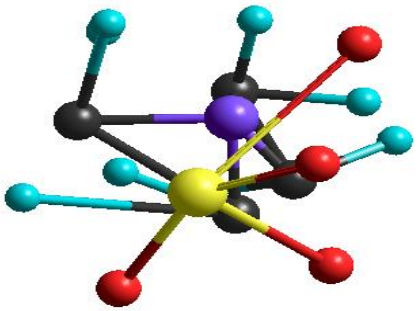


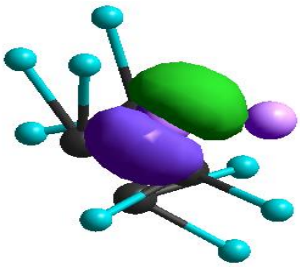
Figure 1. Optimized structure in the cylinder shape, Color: red is oxygen, cyan is hydrogen, black is nitrogen , gray is carbon, sulfur is yellow

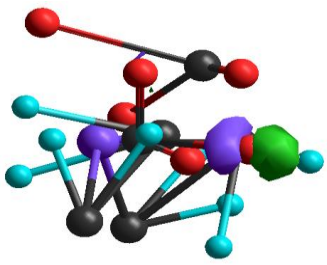
HOMO-LUMO

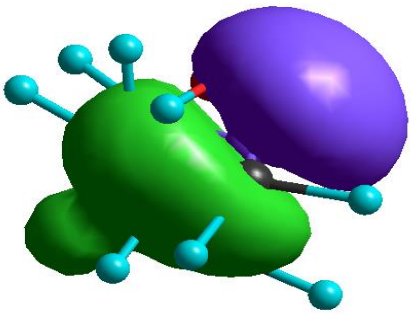
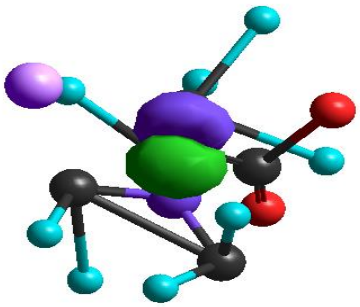
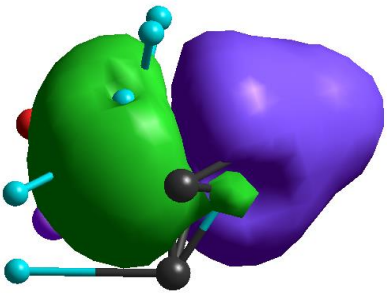
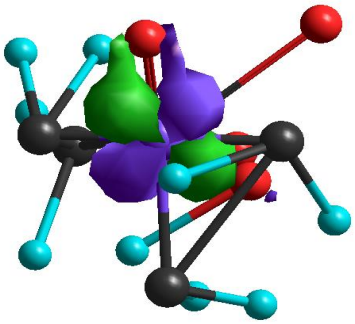
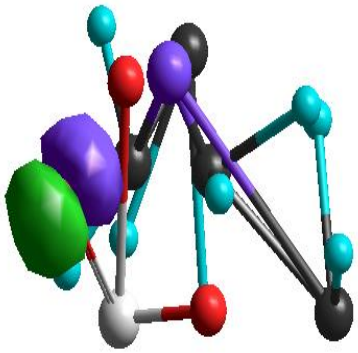
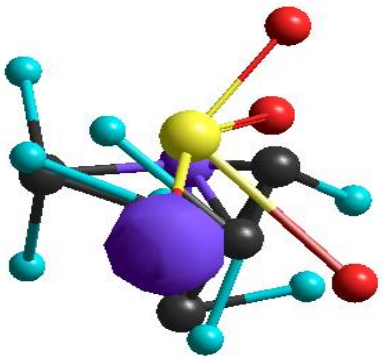
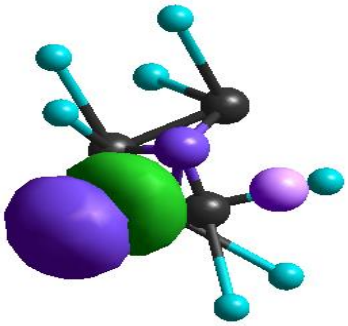
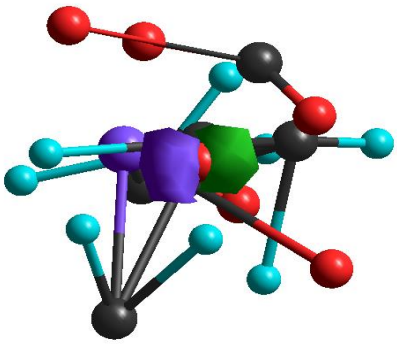
The energy levels of the molecular orbitals order HOMO and LUMO for palladium (II) complexes with different dihydrazine ligands give information on the possible electronic transition. The HOMO and LUMO also indicate the electrophilic and nucleophilic attraction region in the molecule. The LUMO-HOMO gap is the most important parameter for chemical reactivity. The shorter LUMO- HOMO gap is considered as the high reactivity, they are highlighted in Figure 2 colored green is 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 electron.

L01 L02

HOMO





	L03	L04
		
	L05	L06
		
	L07	L08
		
	L01	L02
LUMO		

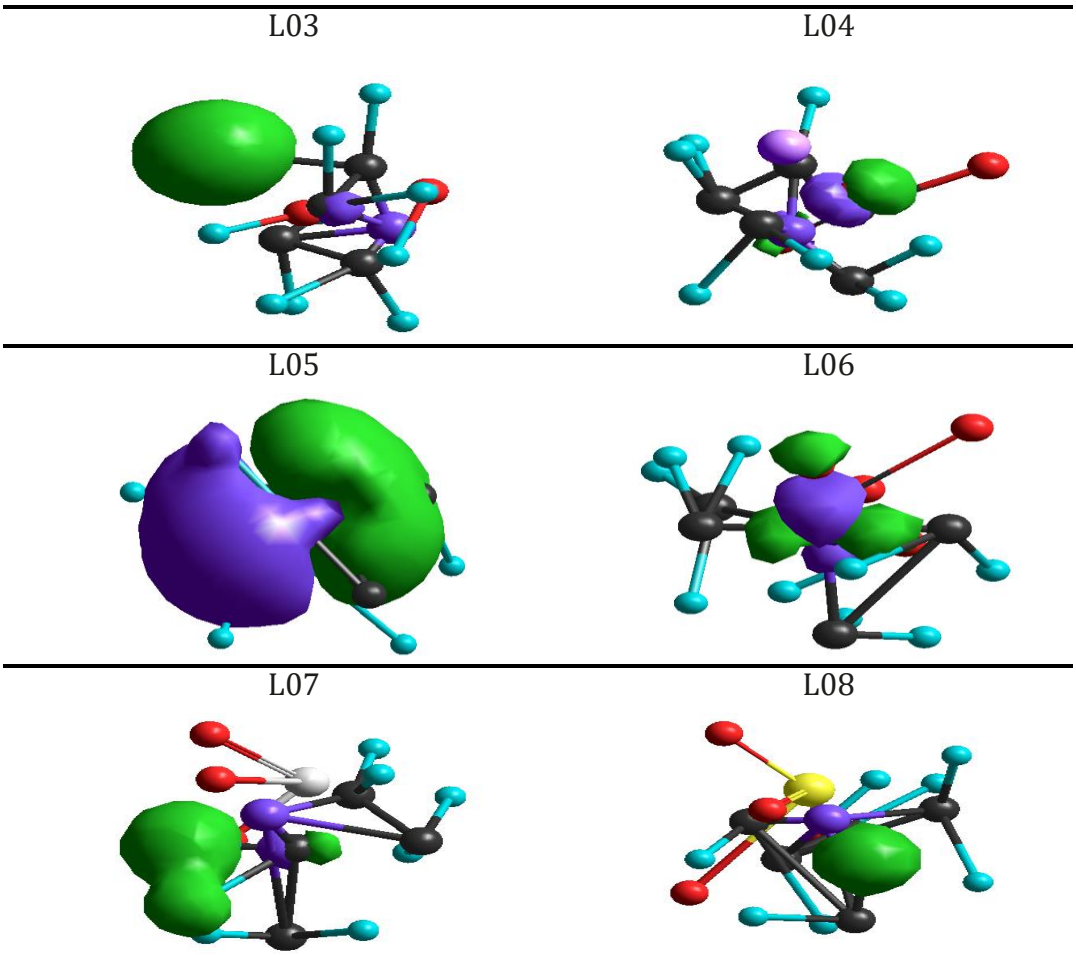


Figure 2. The frontier orbitals: a) HOMO and b) LUMO

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 energy gap which is an important parameter that determines the stability of the structures. The HOMO, LUMO, IP, EA, HOMO-LUMO gap are listed in Table 1.

Table 1. Data for HOMO, LUMO, IP, EA, and LUMO- HOMO gap (ΔE)

	L01	**L02**	**L03**	**L04**	**L05**	**L06**	**L07**	**L08**
HOMO, (eV)	-10.221	-7.116	-5.420	22.370	32.248	31.792	-3.173	-5.359
LUMO, (eV)	-10.089	-6.690	-3.180	23.135	37.717	31.852	-0.261	0.621
Δ_E, (LUMO-HOMO) gap	0.132	0.426	2.240	0.765	5.469	0.059	2.173	5.980
Ionization potential (I),eV	10.221	7.116	5.420	-22.370	-32.248	-31.792	3.173	5.359
Electron affinity (A),eV	10.089	6.690	3.180	-23.135	-37.717	-31.852	0.261	-0.621

The hardness and softness are the most important parameters of chemical stability and Fukai Index. The Fukai index is also considered as the biological activity of molecules. On the other hand, the chemical polarizability is related to the chemical hardness and softness which prescribes the charge population and electronic transition state in the chemical reaction or molecule. The minimum polarizability and minimum hardness indicate the more stable situations of the molecule. The transition state which is least stable is also often associated with higher polarizability and the corresponding trends of higher hardness for higher stability.

Although in general, higher stability indicates higher hardness and lower polarizability, there are exceptions in the trend of both these quantities.

From the Table 2, it is found that the SO_4^{2-}, CO_3^{2-} ions indicate the lower polarizability and higher stability. On the other hand, homo anions like L01 and L02 are less stable almost than other.

Table 2. Biological Indices and chemical kinetics

	L01	**L02**	**L03**	**L04**	**L05**	**L06**	**L07**	**L08**
Hardness, (η)	0.066	0.213	1.120	0.383	2.735	0.029	1.456	2.99
Softness (S)	15.152	4.694	0.893	2.610	0.365	34.483	0.686	0.334
Electrophilicity (ω)	781.319	111.857	8.254	675.84	223.731	17459.30	1.012	0.938
Chemical potential (μ)	-10.155	-6.903	-4.30	22.753	34.983	31.822	-1.717	2.369
Electronegativity, (χ)	10.155	6.903	4.30	-22.753	-34.983	-31.822	1.717	-2.369
Polarizibility, $Å^3$	7.82	8.78	5.10	8.30	6.46	6.94	6.25	5.47

Thermophysical properties

Entropy and enthalpy is an important part of thermodynamics, which allows physics and physical chemistry to participate in any system. 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 temperature, the value of entropy of all the optimized molecules is zero. As a result there are no substances in the zero temperature, no substances in any system and will easily participate in the biochemical chemical reaction. Table 4 is shown that the increase of temperature is mentioned the increase of entropy. That means that the effect of temperature above that system for the reaction occurring is decreased.

On the other hand, binding energy is an important parameter for biological activity studies. As far as the energy level is low, it is considered to be biologically active. In bioactive case, the value of binding energy is negative. If the value of binding energy is more negative, the greater the biological activity of the molecules. When the value of binding energy is positive, the molecules can be considered to be stable. The smaller value of which will be less stable. From table-3 shows that the value of L02 and L04 is very close, and the values of L04, L05, L06, and L08 are between 30000 to 33000 (kcal/mol).

Table 3. Thermophysical properties

Properties	L01	L02	L03	L04	L05	L06	L07	L08
Total energy, (kcal/mol)	-44830.2938	-64438.7308	-44330.97386	-63290.3834	-36198.9345	-58674.0811	-43065.4275	-61192.2889
Entropy, (kcal/mol-deg)	0	0	0	0	0	0	0	0
Free energy, (kcal/mol)	-44830.2938	-64438.7308	-44330.97386	-63290.3834	-36198.9345	-58674.0811	-43065.4275	-61192.2889
Heat capacity, (kcal/mol-deg)	0	0	0	0	0	0	0	0
Dipole moment, (D)	0	0	0	0	0	0	0	0
RMS gradient, (kcal/mol)	976.4	1346	1566	1263	929.1	567.4	841.3	832.9
Binding energy, (kcal/mol)	20458.2241	57785.2650	23787.69831	30465.8771	30504.6581	36497.2740	38454.0869	33662.7895
Heat of formation, (kcal/mol)	21475.0201	59327.4350	24969.8314	31.745.3601	31604.1251	37859.4280	39762.4699	34926.2415
Electronic energy, (kcal/mol)	-190082.523	-381638.2566	-210330.1165	-297400.9719	-146034.9793	-210948.9813	-203253.3103	-256595.3189
Nuclear energy, (kcal/mol)	145252.2291	317199.5185	16599.1426	234110.5884	109836.0448	152274.9201	160187.8828	195403.0291

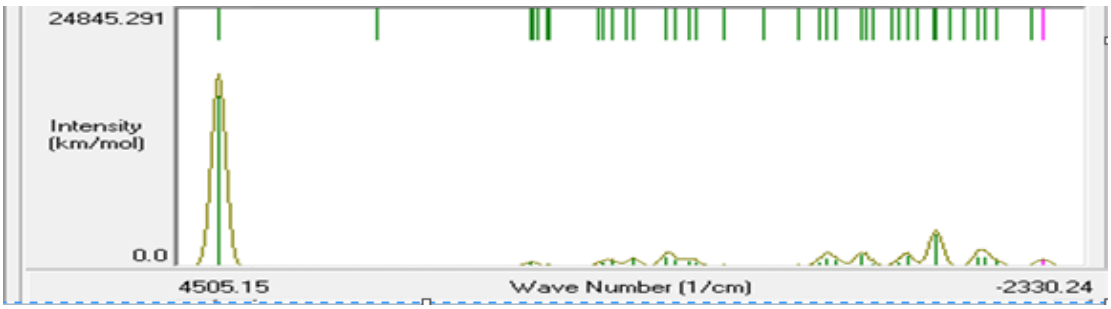
Table 4. Entropy and heat capacity in different temperature

	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	0.0755	0.0129	0.0769	0.0138	0.0782	0.0148
L02	0.0781	0.0154	0.0797	0.0169	0.0813	0.0183
L03	0.0703	0.0105	0.0714	0.0111	0.0725	0.0118
L04	0.0815	0.0180	0.0833	0.0192	0.0851	0.0205
L05	0.0755	0.0151	0.0770	0.0164	0.0786	0.0177
L06	0.0827	0.0196	0.0847	0.0211	0.0866	0.0266
L07	0.0750	0.0128	0.0763	0.0139	0.0777	0.0149
L08	0.0799	0.0168	0.0816	0.0181	0.0833	0.0894

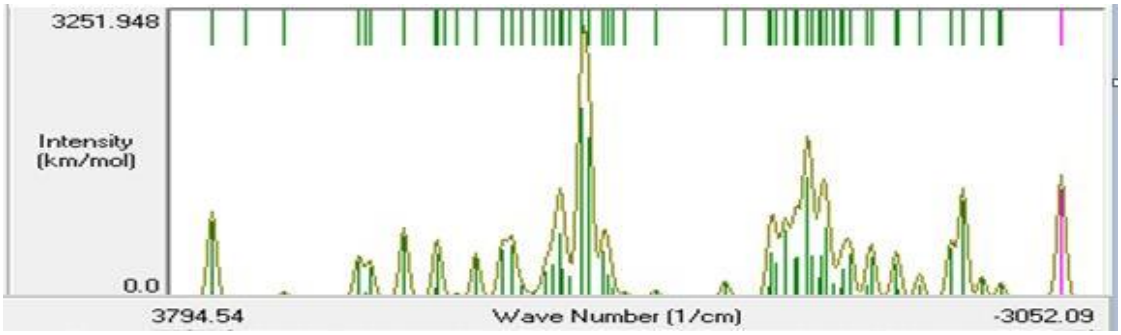
Vibrational spectrum

The vibrational spectrum is the characteristic peak of any molecule for identification similar to the peak. To optimize these molecules for vibrational peak obtain the identified peak in different region about -2300 to 4500 cm^{-1} at which the main characteristic peak of diamine palladium(II) complex is almost 3525- 2300 cm^{-1} represented in Figure 3.

L01



L02



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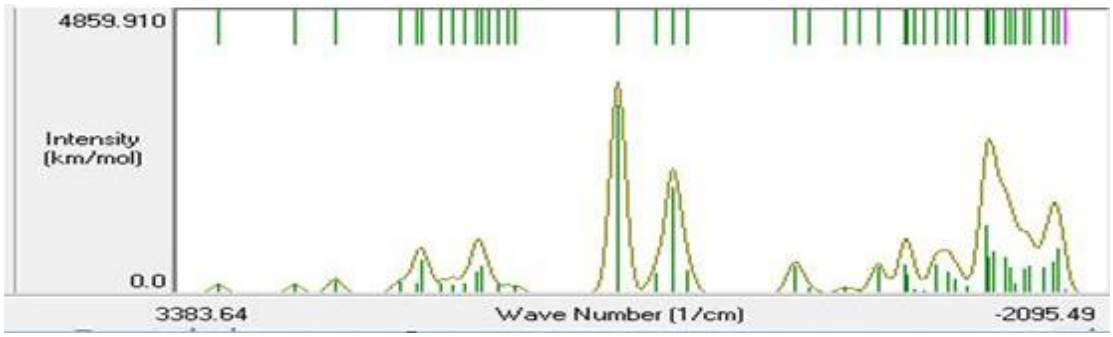
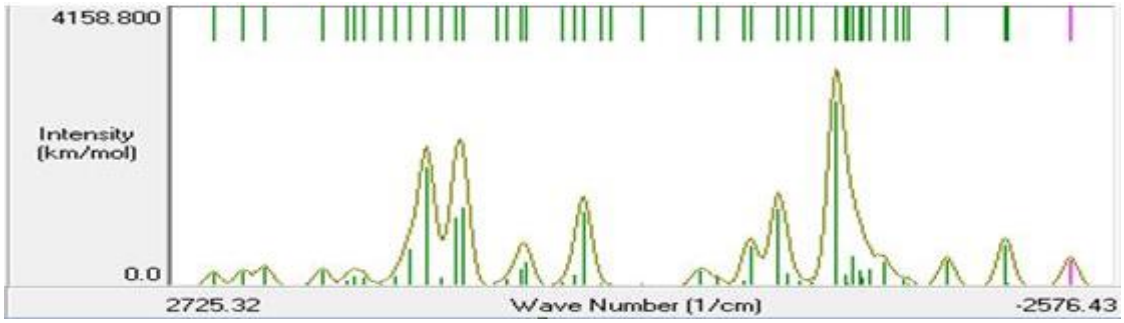
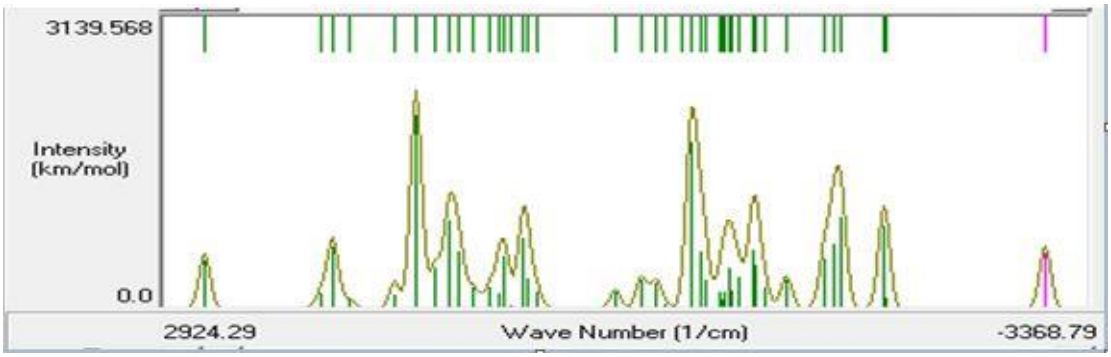


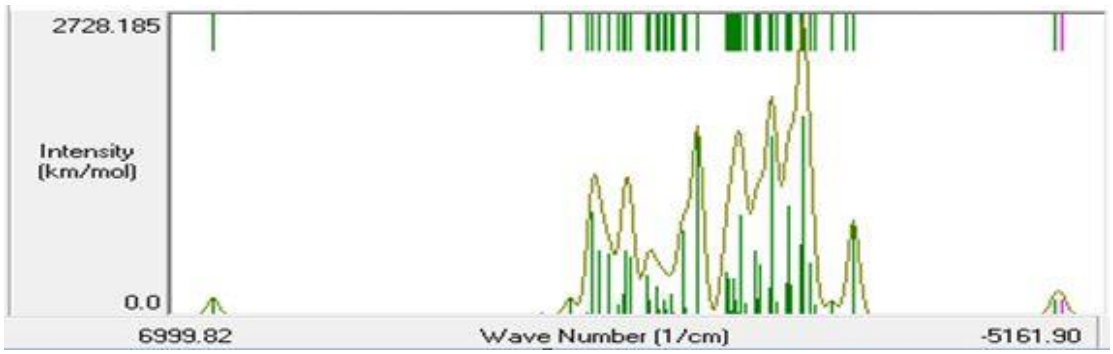
L04



L05



L06



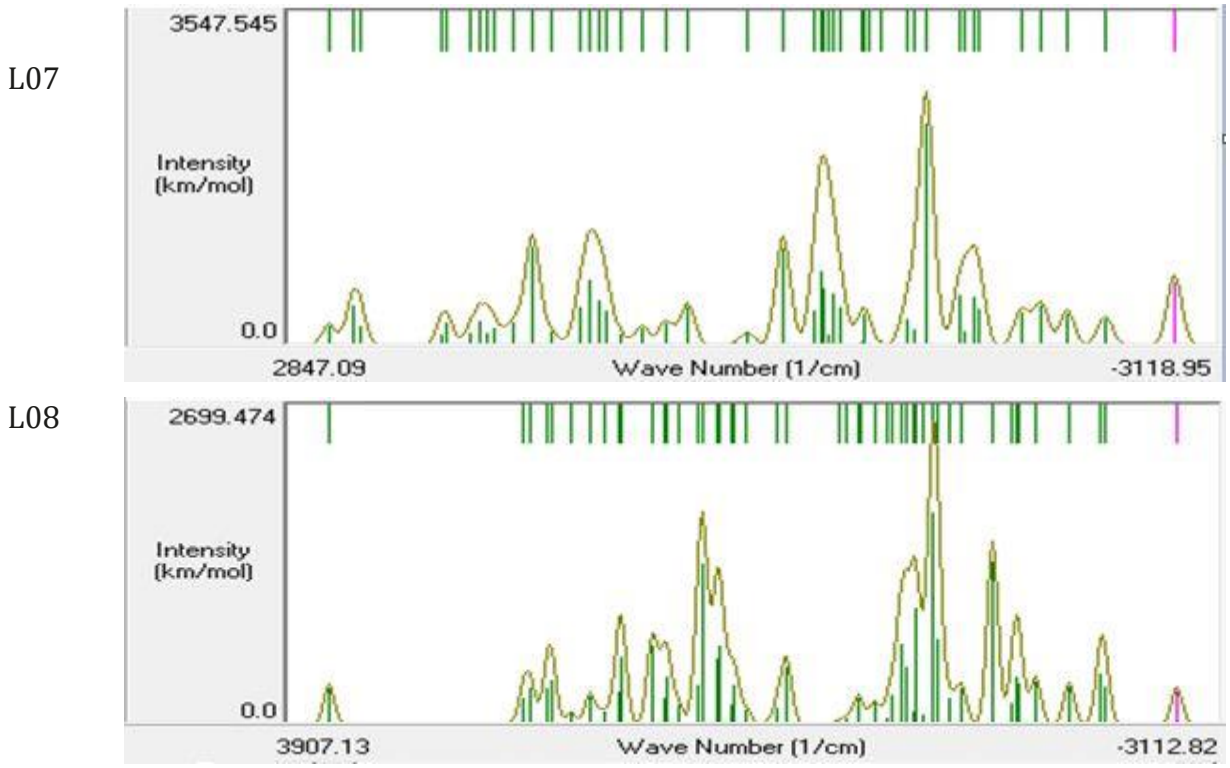


Figure 3. Vibrational spectrum

In the calculation of vibrational spectrum, the condition of normal mode, degeneracy, frequency, intensity and symmetry are used as an independent variable these are given in Table 5.

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

	Normal Mode	Degeneracy	Frequency	Intensity	Symmetry
L01	1	1	-2019.54	656.50	1 A
L02	1	1	-2047.88	1259.79	1 A
L03	1	1	-1846.44	85.65	1 A
L04	1	1	-2335.54	393.47	1 A
L05	1	1	-3082.74	606.16	1 A
L06	1	1	-4609.09	151.59	1 A
L07	1	1	-2847.76	666.40	1 A
L08	1	1	-2793.73	283.03	1 A

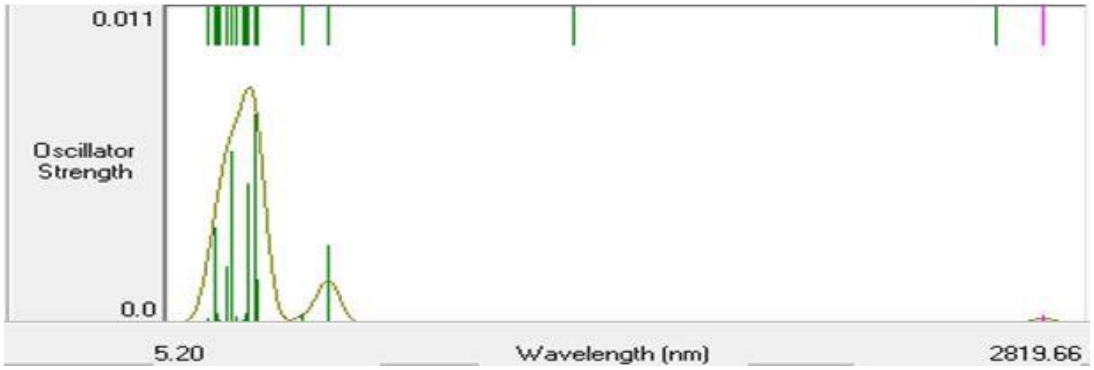
UV-visible spectrum

UV-visible Spectrum provides a powerful technique by which the nature of metalligands bonding may be identified. A remarkable covalence 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

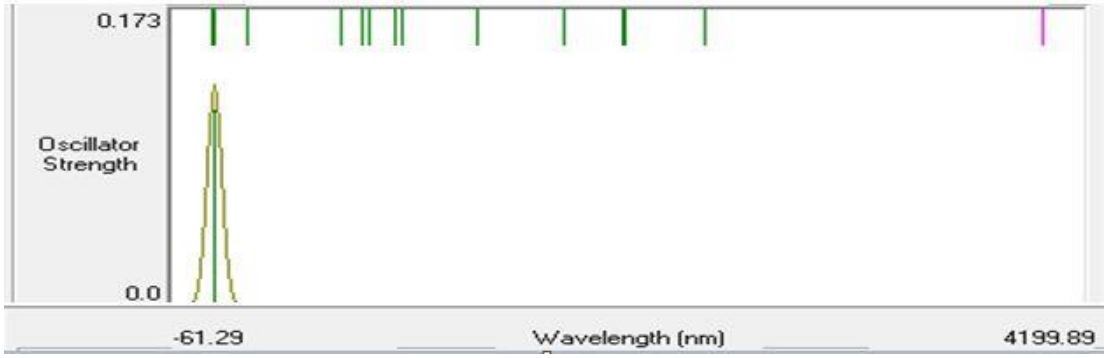
empty 4dxy and 5s metal orbitals and result in important ligand-to-metal charge transfer (Canadell *et al.*, 1990).

The UV-visible spectrum of the diamine palladium(II) complex shows a strong transition near 135 and 170-200 nm, as well as an ultraviolet band of weaker intensity after 250 nm which is shown in Figure 4.

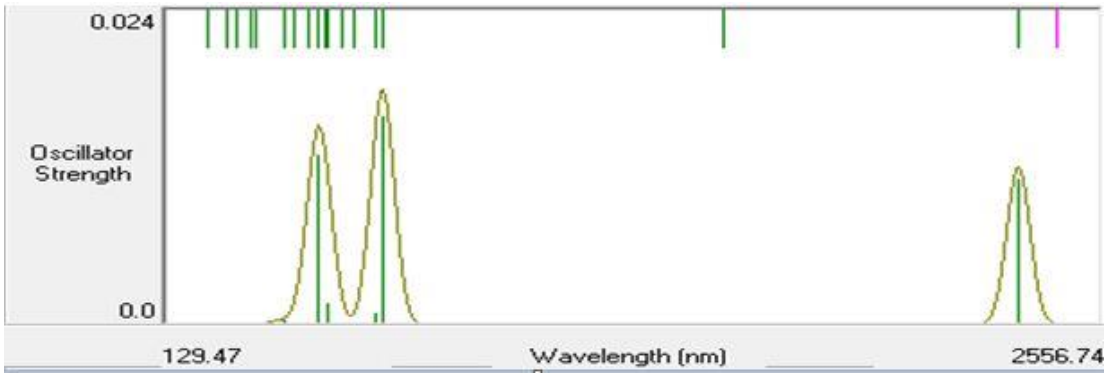
L01



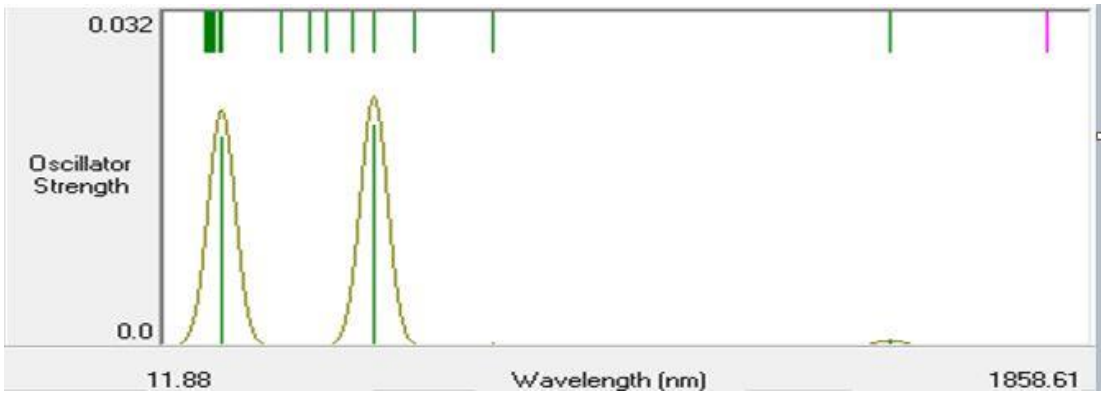
L02



L03



L04



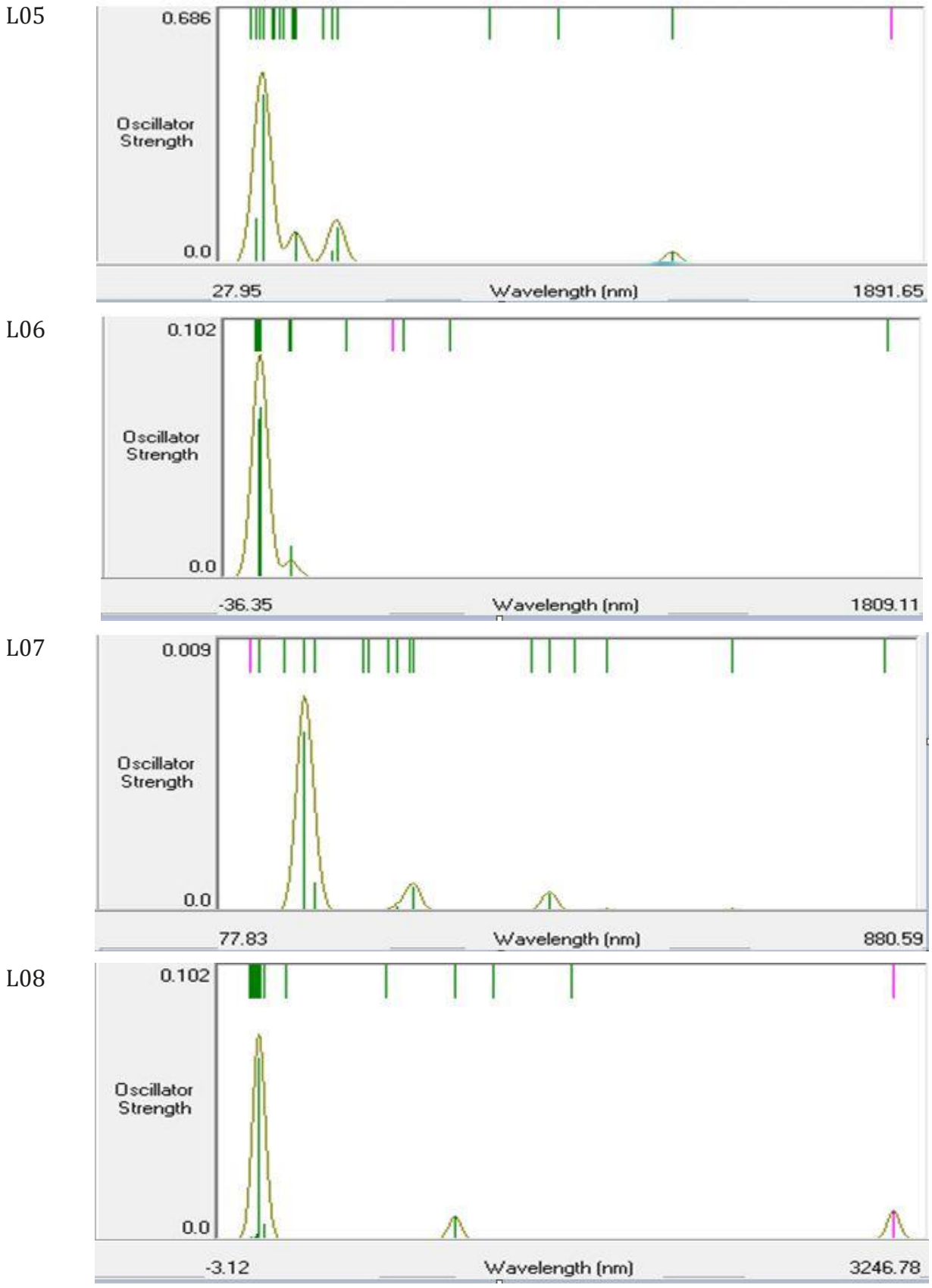


Figure 4. UV-visible spectrum

In the similar way of calculation the UV visible spectrum, some independent variables are related for simulation given Table 6 such as transition state which indicates the electron moving from energy level. On the other hand, degeneracy and spin multiplicity are the important for d- orbital splitting. In the Table 6 also mentions the wavelength and oscillation strength.

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	Singlet	2691.73	0.0
L02	1	1	Singlet	4006.20	0.0
L03	1	1	Singlet	2446.41	0.0
L04	1	1	Singlet	1774.67	0.0
L05	1	1	Triplet	1806.94	0.0
L06	1	1	Triplet	412.83	0.0
L07	1	1	Triplet	114.32	0.0
L08	1	1	Triplet	3099.05	0.0

Biological activity of optimized molecules

The distribution electrostatic potential due to 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 7. This difference, ΔE represents the electronic excitation energy which is possible in a molecule. The electrostatic potential in view of the 3D mapped structure 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 (Böhm *et al.,* 1999).

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(Timofeeva and Kleshcheva, 2011). 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, L04, L05, L06 are highly positive and L03, L07 and L08 are negative, shown in Figure 5 and which play a role in their coupling to different structures in which the complexes are positively charged more in whole surface area.

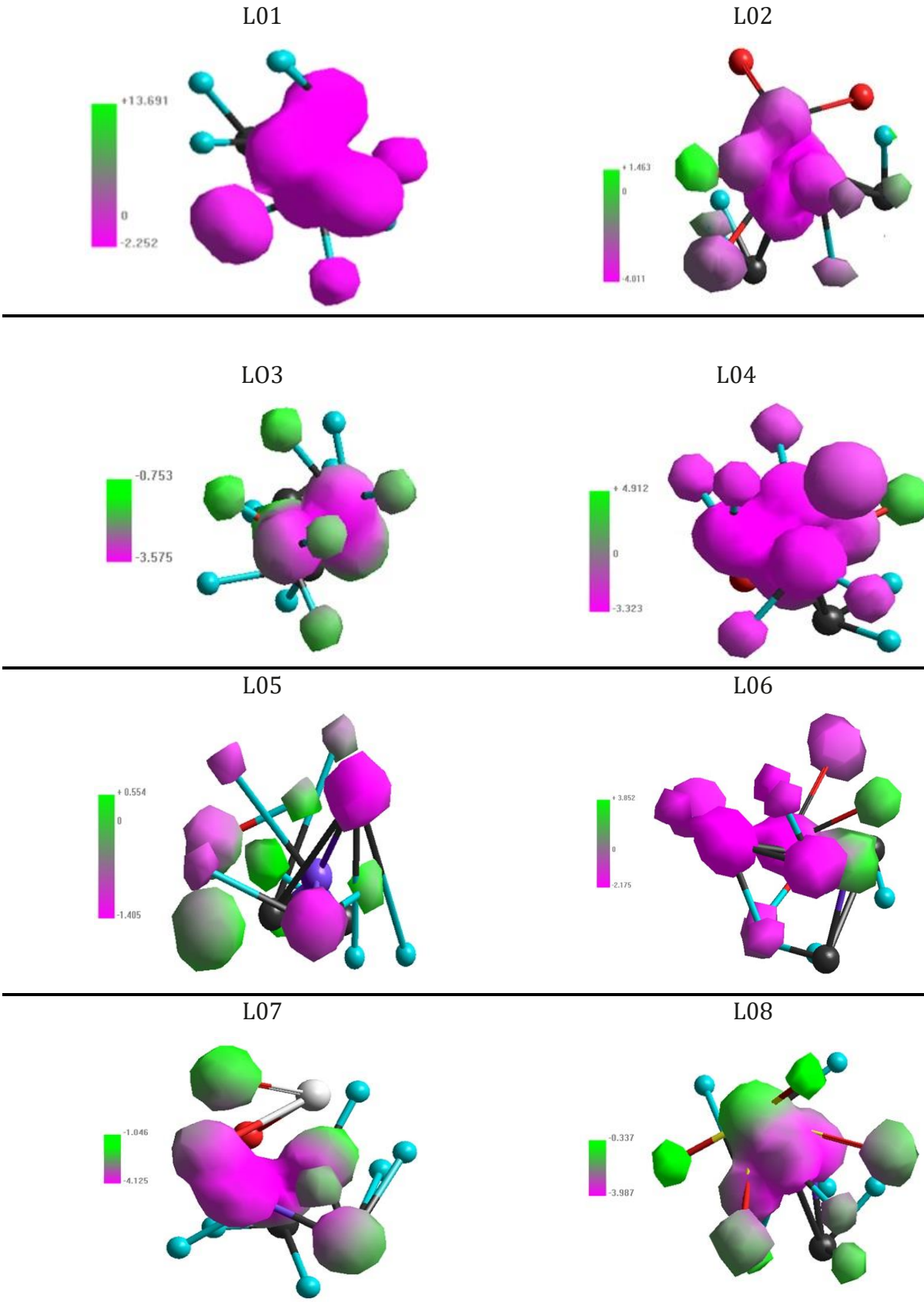


Figure 5. The 3D geometry of the distribution electrostatic potential

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

	L01	L02	L03	L04	L05	L06	L07	L08
E1	+13.69 1	+1.463	-0.753	+4.912	+0.554	+3.852	-1.046	-0.337
E2	-2.252	-4.011	-3.575	-3.323	-1.405	-2.175	-4.125	-3.987
ΔE= E2-E1	-15.943	-5.474	-2.822	-8.235	-1.959	-6.027	-3.079	-3.650

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

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. 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, L04, L05 and L06 complexes are hydrophilic and less toxic. The L07 and L08 are hydrophobic in nature and indicate the higher toxic in views of LogP and Polarizibility data from Table 8.

Table 8. Data for QSAR study

	L01	L02	L03	L04	L05	L06	L07	L08
Partial charge, (e)	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.0
Surface Area(grid),	375.32	468.07	385.81	417.81	480.52	463.82	413.73	460.60
Volume, $Å^3$	577.99	769.96	570.45	652.67	731.58	735.64	659.60	733.30
Hydration Energy kcal/mol	-4.38	-10.48	347.37	-0.86	-1624.40	-26.30	-23.77	-394.95
Log P	-1.34	-0.96	-0.10	-1.15	-0.72	-0.53	0.66	0.22
Refractivity $Å^3$	18.67	21.06	11.89	19.87	15.28	16.48	15.23	18.93
Polarizibility, $Å^3$	7.82	8.78	5.10	8.30	6.46	6.94	6.25	5.47
Mass (amu)	241.40	294.50	204.51	267.95	222.95	249.50	230.50	266.50

Correlation and comparison study in case of different anion with binuclear diamine ligands

In the case of chemical reactivity, the LUMO-HOMO gap in presence of L05, and L08 is almost the same means that with the sulfate ion can show high reactivity. The chemical reactivity is changed poorly for other groups of homogeneous and heterogeneous anions shown in Figure 6.

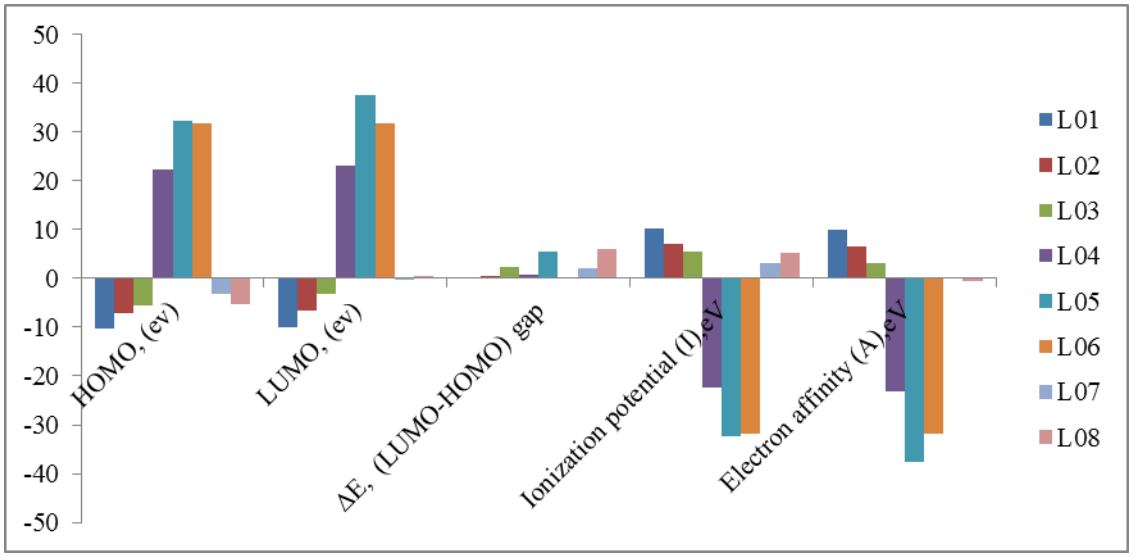


Figure 6: Chemical reactivity relationship

The most important comparison in thermophysical properties is explained that with variety of anions of ligands show variety thermophysical properties listed in Figure 7 that the total energy, binding energy, free energy, heat of formation, and electronics energy are in almost regular pattern.

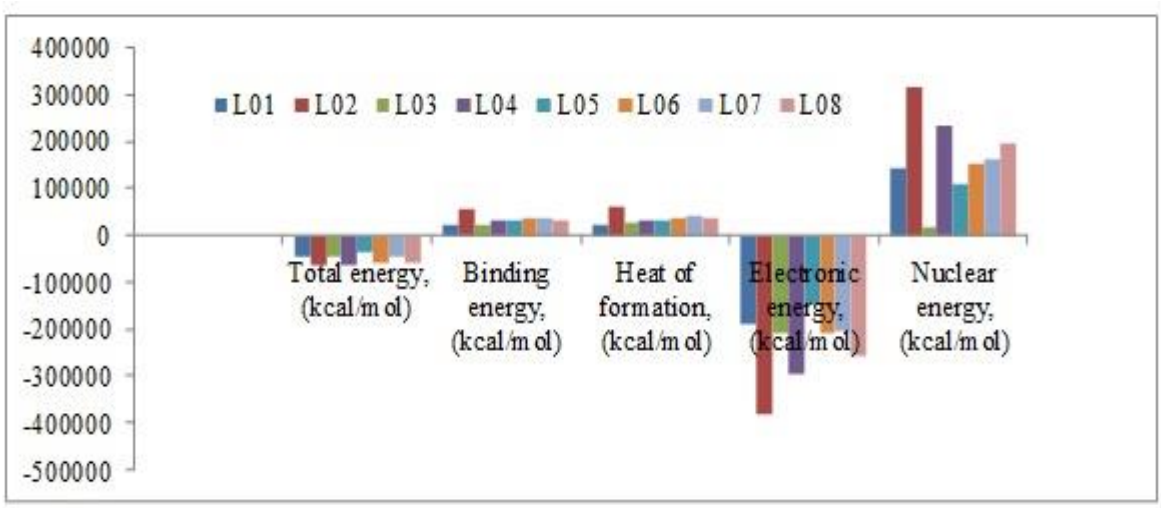


Figure7. Comparison of thermophysical properties

From the Figure 8, it was found that the polarizibility are in nearing to same pattern where the electronegativity of L01, L02 and L03 are positive and others are opposite with about double magnitude. The relationship in chemical potential is same of electronegativity but opposite in case of magnitude. In case of softness and hardness are found almost same activity without L01 and L06.

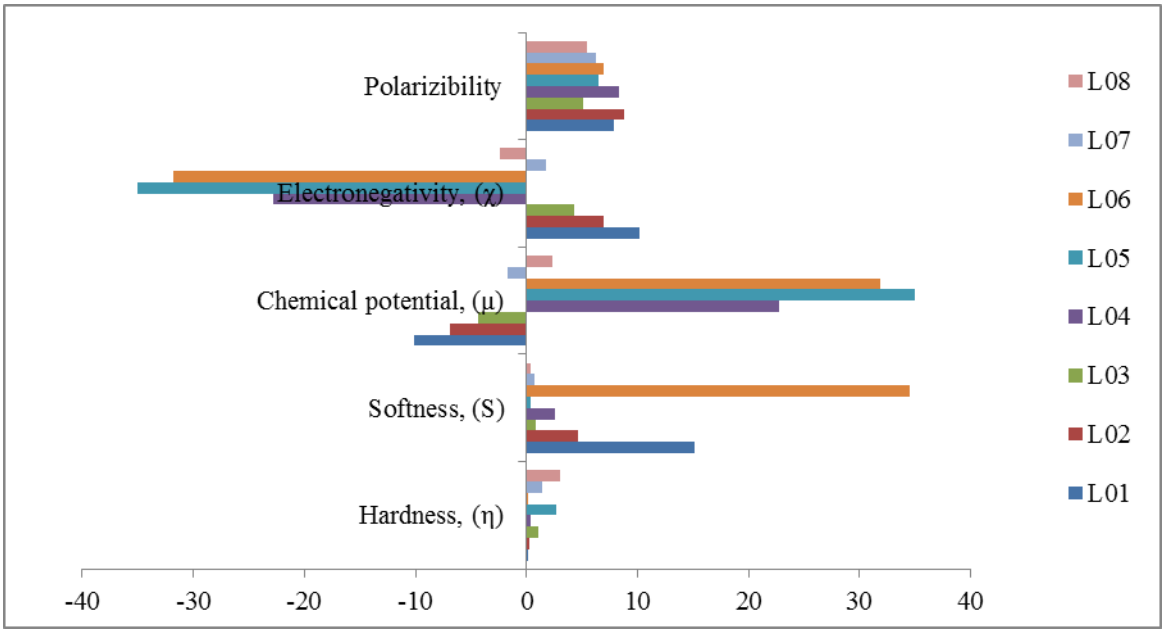


Figure 8. Comparison of chemical and biochemical reactivity

In case of QSAR study which is given in Figure 09 as a comparative study for optimized palladium(II) complexes, the LogP have negative value exception L07 and L08 that is why they are hydrophilic nature and tend to low toxicity.

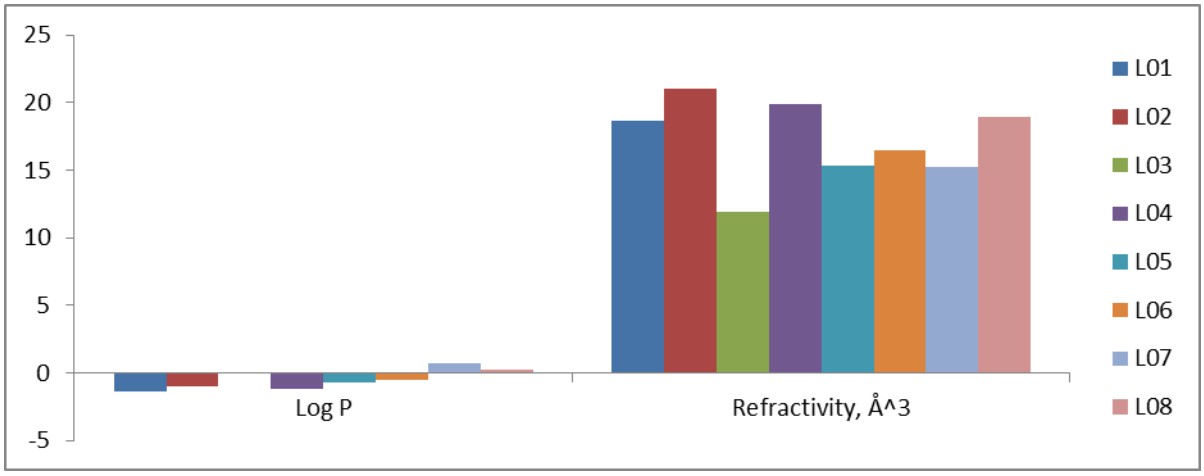


Figure 9. Comparison of QSAR study

Conclusion

The DFT method was used to characterize and optimize of palladium(II) complex with binuclear amine ligands and different anions. Using DFT, the thermophysical, chemical and biological properties were computed. From the spectroscopy studies, the vibration, degeneracy, symmetry, and splitting of d orbitals give the information in an analytical method. In the case of HOMO, LUMO, and HOMO, LUMO gap can be informed that palladium(II) complex with binuclear amine ligands is chemically reactive for further uses.

As the value of LogP is negative, palladium(II) complex with binuclear amine ligands are hydrophilic nature that is why the toxicity is very less and supports the safe uses in all areas. From the evaluated statistical data, the relationship was developed.

Disclosure statement

No potential conflict of interest was reported by the authors.

References

Böhm, M., Stürzebecher, J., and Klebe, G. (1999). Three-dimensional quantitative structure–activity relationship analyses using comparative molecular field analysis and comparative molecular similarity indices analysis to elucidate selectivity differences of inhibitors binding to trypsin, thrombin, and factor Xa. *J. Med. Chem.,* 42:458-477.

Canadell, E, Ravy, S, Pouget, JP, Brossard, L. (1990). Concerning the band structure of D (M (dmit) 2) 2 (D= TTF, Cs, NMe4); M= Ni, Pd) molecular conductors and superconductors: Role of the M (dmit) 2 Homo and Lumo. *Solid State Commun.,* 75:633-638.

Chen, X, Engle, KM, Wang, DH, Yu, JQ. (2009). Palladium (II), catalyzed C, H activation/C, C cross, coupling reactions: versatility and practicality. *Angew. Chem. Int. Ed. Engl.,* 48:5094-5115.

Doucet, H, Hierso JC. (2007). Palladium coupling catalysts for pharmaceutical applications. *Curr. Opin. Drug Discovery Develop*., 10:672-690.

Garrett, CE, Prasad, K. (2004). The art of meeting palladium specifications in active pharmaceutical ingredients produced by Pd-catalyzed reactions. *Adv. Synth. Cataly.,* 346:889-900.

Hossain, MI, Kumer, A. (2018). Synthesis and Characterization of Ammonium Ionic Liquids and Their Antimicrobial and Computational Overview. *Asian J. Chem. Sci.,* 3:1-10.

A Howard, J. McIver and J. Collins, "HyperChem Computational Chemistry," Publishing HC40-00-03-00, Hypercube Inc., Waterloo/Ontario/Canada, 1994.

Koopmans, YT. (1934). Uber die zuordnung von wellenfunktionen und eigenwerten zu den,einzelnen elektronen eines atoms. *Physica*, 1:104-113.

Kumer, A, Ahmed, B, Sharif, MA, Al-Mamun, A. (2017). A Theoretical Study of Aniline and Nitrobenzene by Computational Overview. *Asian J. Phys. Chem.* Sci., 4:1-12.

Kumer, A, Sarker, N, Paul, S. (2019). The theoretical investigation of HOMO, LUMO, thermophysical properties and QSAR study of some aromatic carboxylic acids using HyperChem programming. *Int. J. Chem. Technol.,* 3:26-37.

Kumer, A, Sarker, N, Paul, S, Zannat A. (2019b). The Theoretical Prediction of Thermophysical properties, HOMO, LUMO, QSAR and Biological Indics of Cannabinoids (CBD) and Tetrahhdrocannabinol (THC) by Computational Chemistry. *Adv. J. Chem. A,* 2:190-202.

Lazarević, T, Rilak, A, Bugarčić, ŽD. (2017). Platinum, palladium, gold and ruthenium complexes as anticancer agents: Current clinical uses, cytotoxicity studies and future perspectives. *Eur. J. Med. Chem*., 142:8-31.

Miyaura, N, Suzuki, A, (1995). Palladium-catalyzed cross-coupling reactions of organoboron compounds. *Chem. Rev.,* 95:2457-2483.

Miyaura, N, Yanagi., T, Suzuki, A. (1981). The palladium-catalyzed cross-coupling reaction of phenylboronic acid with haloarenes in the presence of bases. *Synth. Commun.,* 11:513-519.

Ray, S, Mohan, R, Singh, JK, Samantaray, MK, Shaikh, MM, Panda, D, Ghosh, P. (2007). Anticancer and antimicrobial metallopharmaceutical agents based on palladium, gold, and silver N-heterocyclic carbene complexes. *J. Am. Chem. Soc.,* 129:15042-15053.

Timofeeva, L, Kleshcheva, N. (2011). Antimicrobial polymers: mechanism of action, factors of activity, and applications. *Appl. Microbial. Biotechnol*., 89:475-492.

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