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Study of Electronic Transition of Complex Fe(III), Ni(II) and Zn(II)-1,10-Phenanthroline: Modelling and UV-Vis Spectral Analysis

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Abstract: Geometric modeling and geometric optimization of Fe(III)-1,10-phenantroline (Fe-Phen), Ni II)-1,10-phenantroline (Ni-Phen) and Zn(II)-1,10-phenantroline (Zn-Phen) compounds have been carried out computing using the semi-empirical method of PM3. The spectral measurements and the study of complex electronic compositions using the UV-Vis spectrophotometer and simulation of ZINDO/s (Zerner's Neglect of Differential Overlap) calculations. The optimum result of the geometry of complex molecule found there is a change of charge in each complex with stable energy. The UV-Vis spectra measurements showed λmax in the Fe-Phen complex: 315.50 nm, Ni-Phen complex: 325.00 nm and Zn-Phen complex: 315.00 nm. The electronic transition occurring at these three complexes shows the transition characteristics of electrons at the level of the molecular orbitals π to π^* and the degree of the molecular orbitals n to $\overset{*}{\pi}$. Electron transition energy in complex orbital molecules can be observed in the energy changes of each molecular orbitals.

Keywords: 1,10-phenanthroline, complex ion, semi-empirical method, zindo/s.

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INTRODUCTION

The complex compounds have molecular structures composed of ligands/complexes binding in coordination with metal ions as the center of the molecular geometry of complex compounds (1). Generally, metal ions of complex compounds/ions are derived from transition metals having neutral or positive oxidation numbers (2). For example, Fe(III), Cu(II), Co(II), Mn(II), Zn(II), and Ni(II) are employed as other metals. Metals are often reacted with complexes/ligands having neutral or negative oxidation numbers to obtain complex compounds/ions (3). Examples of ligands/complexes binding to heavy metals in the form of ions, ie, 1,10-phenanthroline, EDTA, pyrazinamide, pyridine, and ligand/other complexes. Generally, complex compounds have many benefits in the world of health and materials science (4). In addition has been investigated the influence the use of 1,10-phenanthroline ligand with Co(II) metal ions on DNA binding, cleavage, and anticancer properties showed good results (5). The ligand 1,10-phenanthroline often used in complex compounds because it's exhibit good ability to coordinate bonds with metal ions (6). Ion of Fe(III), Ni(II) and Zn(III) are ions of transition metals that can form complexes with ligand 1,10-phenanthroline (7, 8). Interaction between metal ions with two lone pairs electrons in ligand 1,10-phenanthroline forms complexes bound to coordinate with different molecular geometries (9, 10).

Electron transitions that occur in ligands and complex compounds can be calculated using a UV-Vis spectrophotometric analysis (11). The transition of electrons to complex compounds occurs at the level of their molecular orbital with the most urgent electron excitation being σ to $\overset{*}{\sigma}$ and the electron excitation requiring the least energy is n to $\overset{*}{\pi}$. The occurrence of electron transfer from the lowest ground state energy (HOMO) to the excited energy level (LUMO) can be known by its wavelength uptake. Ligands 1,10-phenanthroline and ligand to ligand change transfer (LLCT) undergo electron transition in orbital molecules (OM) level π to $\overset{*}{\pi}$ (12). In the meantime, ligands and complex compounds containing nitrogen atoms (RC = N) have an electron transition at OM level n to $\overset{*}{\pi}$ (13).

Modeling of complex ion has been done using the method of semi-empirical ZINDO/s to analyze the electronic and energy transitions of HOMO and LUMO (14). HOMO and LUMO energy analysis is required as information/reference to know the transfer of charge in a molecule (15). The study of complex molecular modeling aims to facilitate visualization and conducting studies on electronic transition spectra (16, 17, 18). ZINDO / s is one of many semi-empirical calculation methods in computation that is intended for calculation on UV spectra (19). In addition, it has been known that the method of semi-empirical ZINDO/s was very good at performing electronic transition calculations (20). Thus using the method of semi-empirical ZINDO/s can study geometry and electronic transitions of complexes of Fe (III), Ni (II) and Zn (II) with the 1,10-phenanthroline complex.

EXPERIMENTAL

Measurement of Complex Solutions

In 0.5 mL standard solution, 100 ppm each of $FeCl_3$ (aq), $Ni(NO_3)_2$ (aq) and $ZnCl_2$ (aq) were added 1.5 mL of 1,10-phenanthroline solution at 1000 ppm, 1.5 mL of acetate buffer solution at pH 3.5 and 5 mL of acetone and diluted to a volume of 10 mL with DM water. The Fe-Phen, Ni-Phen and Zn-Phen complexes formed were measured their absorbance using a UV-Vis spectrophotometer.

Optimization of Complex Molecular Compounds

Ligand and complex geometries can be optimized through computational methods (21). Optimization of molecular geometries for Fe-Phen, Ni-Phen and Zn-Phen metal complexes using PM3 (Parameterized Model 3) with a gradient change limit of 0.01 kcal/Å.mol, with gradient boundaries comrade based on the Polak-Ribiere method in the Windows 8 based version of Hyperchem version 8.0.10. The results of the optimization of molecular geometry using the semi-empirical method of PM3 obtain molecular geometry with smaller and stable energy (22).

Complex ion modeling

The modeling of the structure of the geometric optimization results from the semi-empirical method of PM3, followed by single point calculation using the method of semi-empirical ZINDO/s to produce electronic transition spectra data. The calculations are done with the limit of configuration interaction (*CI*) and with single excitation (*singly excited-CI*). Spectral calculation data is presented as a discontinuous spectra diagram to analyze the electronic transition.

RESULTS AND DISCUSSION

Complex Ion Modeling

The molecular structure modeling for Fe-Phen, Ni-Phen and Zn-Phen complexes was computed by optimizing its molecular geometry using the semi-empirical PM3 method. Optimization of the molecular geometry of Fe-Phen, Ni-Phen, Zn-Phen and 1,10-phenanthroline ligands using the semi-empirical PM3 method (Figure 1). The geometric optimization results in molecular geometry with the total energy and the smallest or near-zero heat generation energy (Table 1). The total energy value shown in each complex through the simulation of the PM3 method determines how much energy it takes for the interconnected atoms to form a complex molecule (23).

Table 1: Optimization of Complex Molecular Geometry Using the Semi-Empirical Method of PM3

Complex	Total Energy (kcal/mol)	Heat Formation (kcal/mol)
Fe-Phen	-141168.5256	389.0235
Ni-Phen	-109936.3877	275.3654
Zn-Phen	-86813.2124	160.8909

The results of the complexes of Fe(III), Ni(II), and Zn(II) ions with the 1,10-phenanthroline complex produce three complexes with molecular geometry, molecular orbital energy levels, charge and different magnetic properties. The three properties of these molecule complex properties can be reviewed through simulation of geometric optimization of PM3 methods and theoretical approaches (Theory of Molecular Orbital and Hybridization Theory) for the three complex compounds (24).

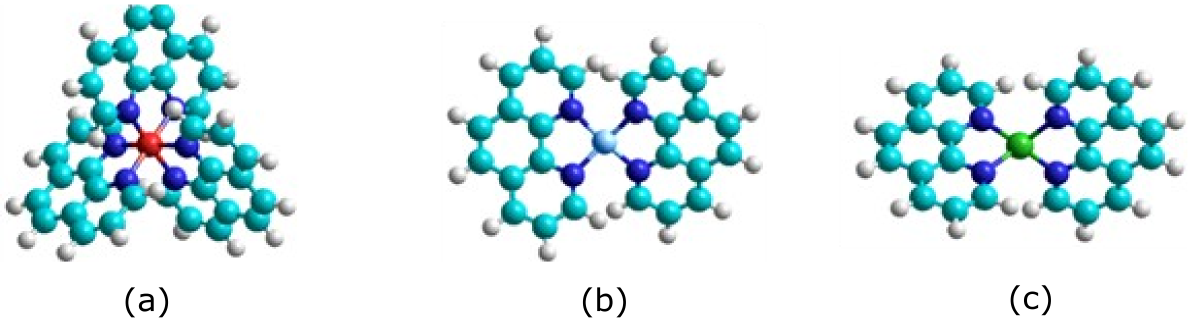


Figure 1. Optimization Geometry of 3D Molecular (a) Fe-Phen, (b) Ni-Phen and (c) Zn-Phen Using PM3.

The calculation of charge and coordinates has been done using the PM3 method to explain how the atoms bind to form the third molecular geometry of the complex. The Fe-Phen complex exhibits a change in values at the coordinates (x, y, and z) of atoms both before and after binding to form a complex (Table 2). The geometry for the Fe-Phen complex forms an octahedron with each ligand (ligand 1: N5' and N11', ligands 2: N19' and N25', 3: N33' and N39' ligands) contributes 2 lone pair electrons to the metal ion (Fe43'). The change in the coordinate value of each bonded atom (Zn') forms the angle of octahedral geometry in the Fe-Phen complex of 90°. The complex Fe-Phen has analyzed with XRD and processed with Rietica program to find the crystallography of the compound. Diffractogram data shows that geometric prediction Fe-Phen was octahedral with monoclinic crystal system, space group C2/c with parameter a = 10.781 Å, b = 24.53 Å, c = 13.286 Å, β = 103.15º and the volume = 3422 Å^3, Rp = 5.37 and Rwp = 11.05 (25).

Table 2: List of Charge (eV) and Coordinates of x, y, z (Å) Fe-Phen PM3

Atom	Charge	x	y	z
N_5	-0.020226	-0.17650	-2.00652	0.00000
N_5'	0.458976	-3.11734	0.60509	-0.43874
N_{11}	-0.020226	-2.65070	-0.60355	0.00000
N_{11}'	0.403515	-1.02197	1.80464	0.57257
N_{19}	-0.020226	-0.17650	-2.00652	0.00000
N_{19}'	0.368995	0.35957	-0.61562	0.46959
N_{25}	-0.020226	-2.65070	-0.60355	0.00000
N_{25}'	0.368761	-1.91295	-0.41832	1.77719
N_{33}	-0.020226	-0.17650	-2.00652	0.00000
N_{33}'	0.459333	-0.83260	0.35945	-1.77590
N_{39}	-0.020226	-2.65070	-0.60355	0.00000
N_{39}'	0.401748	-1.76790	-1.80346	-0.63729
Fe_{43}	3.000000	-1.37339	0.11588	0.00000
Fe_{43}'	-0.616334	-1.40230	0.00614	0.00614

Description: (N) is an atom of a metal-ligand/ion prior to bonding and (N ') is an atom of a metal-ligand/ion after binding.

The change in the coordinate of the Ni-Phen complex forms the planar quadrangle molecular geometry of a central atom attached to a bond angle of 90°. The change of charge value at Ni10 (2.0000) to Ni10' (-1.102833) indicates the occurrence of atoms before and after binding of delocalized electrons and forming a more stable charge to form molecules with a charge value close to the Ni-Phen complex charge value (Table 3). Molecular geometry is formed in the Zn-Phen complex in a tetrahedral geometry. The calculated coordinate using the PM3 method on bonded atoms (N5', N10', N12 ', N21' and Zn11') are coordinated x, y, and z forming a bonding angle of 109.5° (Table 4).

Table 3: List of Charge (eV) and Coordinates of x, y, z (Å) Ni-Phen PM3

Atom	Charge	x	y	z
N_5	-0.020226	-0.17650	-2.00652	0.00000
N_5'	0.709769	-2.55195	0.56285	-0.67382
N_9	-0.020226	-2.65070	-0.60355	0.00000
N_9'	0.709631	-0.58458	1.77623	0.63756
N_{11}	-0.020226	-0.17650	-2.00652	0.00000
N_{11}'	0.709559	0.33598	-0.71135	1.17883
N_{20}	-0.020226	-2.65070	-0.60355	0.00000
N_{20}'	0.709639	-0.76838	-1.42299	-1.13126
Ni_{10}	2.000000	-1.63504	0.74277	0.00000
Ni_{10}'	-1,102833	-0.89210	0.05123	0.00240

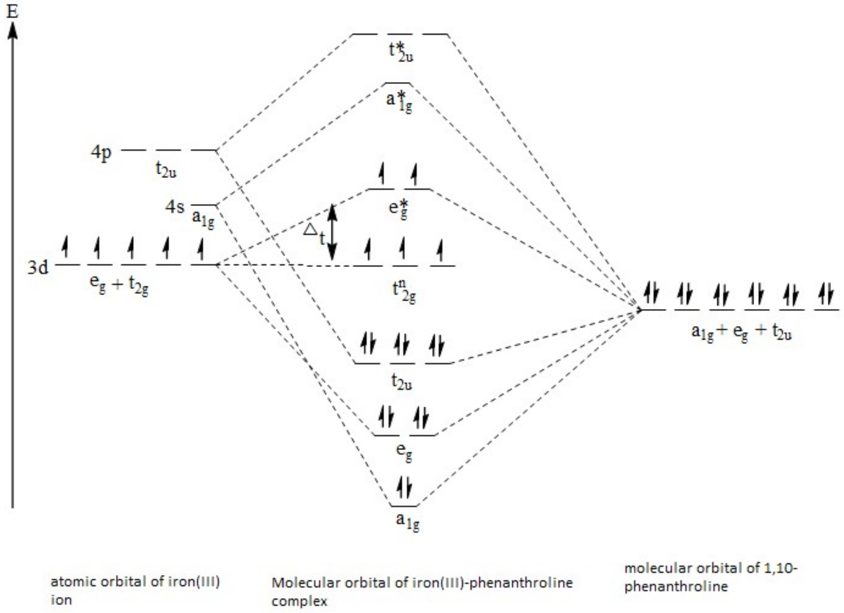
Description: (N) is an atom of a metal-ligand/ion prior to bonding and (N ') is an atom of a metal-ligand/ion after binding.

Table 4: List of Charge (eV) and Coordinates of x, y, z (Å) Zn-Phen PM3

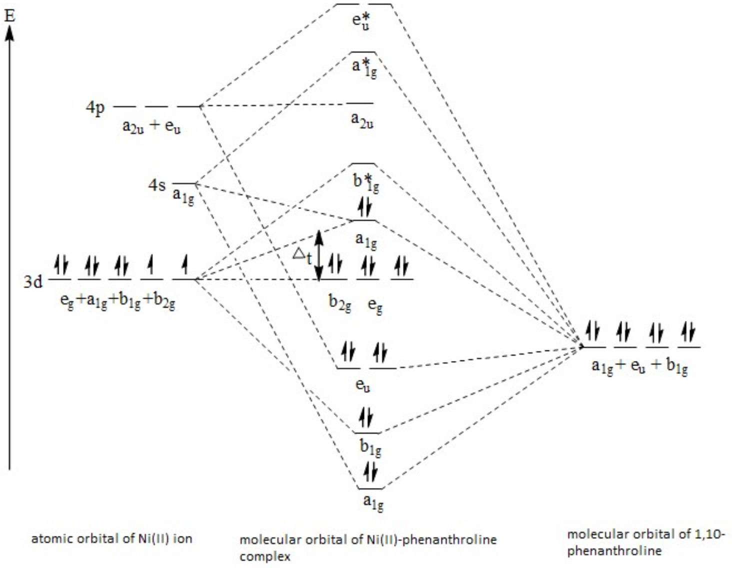
Atom	Charge	x	y	z
N_5	-0.020226	-0.17650	-2.00652	0.00000
N_5'	0.262773	-2.82160	0.58788	-0.17861
N_{10}	-0.020226	-2.65070	-0.60355	0.00000
N_{10}'	0.262542	-0.47977	2.00170	0.18141
N_{12}	-0.020226	-0.17650	-2.00652	0.00000
N_{12}'	0.264556	0.00334	-1.11636	1.37016
N_{21}	-0.020226	-2.65070	-0.60355	0.00000
N_{21}'	0.264380	-0.28653	-1.29103	-1.36826
Zn_{11}	2.000000	-1.32618	0.27897	0.00000
Zn_{11}'	-0.365938	-0.89694	0.04629	0.00118

Description: (N) is an atom of a metal-ligand/ion prior to bonding and (N ') is an atom of a metal-ligand/ion after binding.

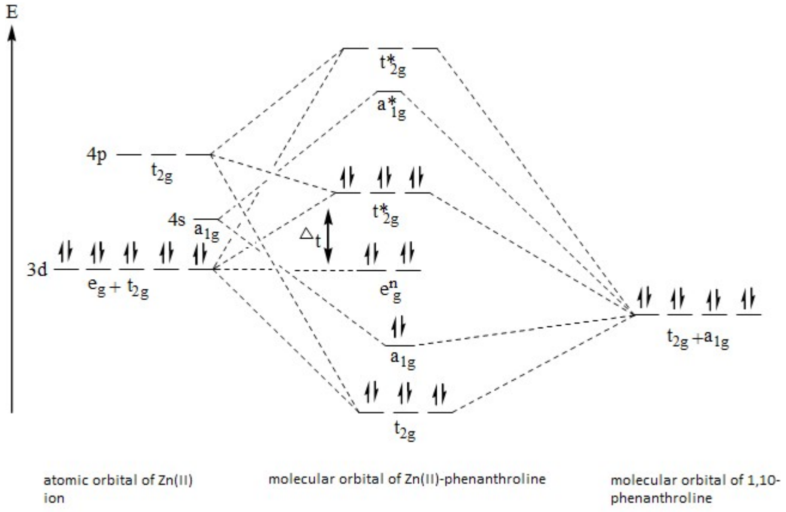
The bonds that occur in the Fe-Phen, Ni-Phen and Zn-Phen complexes can be explained in the theory of hybridization at the level of their molecular orbital. The simulation of the process of complex molecular orbital fusion explains how the new orbitals (hybrids) formed with Fe(III), Ni(II) and Zn(II) metal ions with 1,10-phenanthroline ligands. Hybrid orbitals formed from the three complexes are able to explain the molecular geometry and complex magnetic properties. The Fe-Phen complex forms a d^2sp^3 hybrid orbital, Ni-Phen: dsp^2 and Zn-Phen forming sp^3. The hybridization of these complex molecular orbitals is composed of adjustment of orbital energy to form bonds and produce hybrid orbitals. Based on the filling and position of electrons in complex orbital, it can know the magnetic properties. The Fe-Phen complex is diamagnetic, Ni-Phen is paramagnetic and Zn-Phen is paramagnetic. The orbital interactions are due to the rearrangement of electrons in the orbitals of metal ions with ligands 1,10-phenanthroline. Each ligand of 1,10-phenanthroline binds in coordination with 2 lone pairs electron on Fe(III) forming $[Fe(C_{12}H_8N_2)_3]^{+3}$, Ni(II): $[Ni(C_{12}H_8N_2)_2]^{+2}$ and Zn(II): $[Zn(C_{12}H_8N_2)_2]^{+2}$.


E
t^*_{2u}
a^*_{1g}
4p
t_{2u}
4s
a_{1g}
e^*_g
Δ_t
3d
$e_g + t_{2g}$
t^n_{2g}
t_{2u}
e_g
a_{1g}
$a_{1g} + e_g + t_{2u}$
atomic orbital of iron(III) ion
Molecular orbital of iron(III)-phenanthroline complex
molecular orbital of 1,10-phenanthroline

(a)


E
e^*_u
a^*_{1g}
4p
$a_{2u} + e_u$
a_{2u}
4s
a_{1g}
b^*_{1g}
a_{1g}
Δ_t
3d
$e_g+a_{1g}+b_{1g}+b_{2g}$
b_{2g}
e_g
e_u
b_{1g}
a_{1g}
$a_{1g} + e_u + b_{1g}$
atomic orbital of Ni(II) ion
molecular orbital of Ni(II)-phenanthroline complex
molecular orbital of 1,10-phenanthroline

(b)



(c)

Figure 2. The energy level of the molecular orbital for complexes (a) Fe-Phen, (b) Ni-Phen, and (c) Zn-Phen.

The absorption spectrum of a metal ion produces a change of electron congruity and the maximum wavelength value presented in the measurement value Δ_{oct} (26). Based on the Figure 2 of 5 electrons filling starts from the lowest-energy orbital recall to the highest energy orbitals, ie σ (bond orbital) to n (orbitals not bonded) to σ* (antibonding orbital). The electron configuration of the metal ion lies in the d^n orbital, with the energy level being split into 2 parts, ie eg and t_2g. Configuration of electrons for Fe-Phen: t_2g^3 eg^2 (Δ_{oct} = 0), Ni-Phen: t_2g^6 eg^2 (Δ_{oct}: -1.2) and Zn-Phen: t_2g^6 eg^4 (Δ_{oct}: 0). The division of the d orbital in each complex aims for the adjustment of energy during the electron filling process at the level of the molecular orbital.

Hybridization of molecular orbitals of complex compounds (Figure 2) was the adjustment process in orbital energy to bind and produce hybrid orbital. Based on electron charging and position in an orbital complex, magnetic characteristics can be known. Fe(III)-phenanthroline complex is paramagnetically observed from unpairing orbital electron charging energy so that it has a strong magnetic power, while Ni(II)-phenanthroline and Zn(II)-phenanthroline has a weak magnetic power as it has pairing orbital electron (26, 24). Furthermore, Ni(II) and Zn(II) complexes have a planar and tetrahedral molecule which shows diamagnetic characteristic in complex (11).

Electron charging theoretically based on the theoretical molecular orbital approach in the complex molecules were presented in Figure 2. Electron filling at the orbital level aims to illustrate how the energy adjustments of the orbitals formed from each complex. Meanwhile, to study the electronic transition of each complex is carried out using the ZINDO/s semi-empirical method in the excited state. The computational results, the electronic transition that appear in the ZINDO/s simulation for the Fe-Phen complex of 18 transition peaks indicate the transition types n to π* and π to π*. However, only 3 peaks in the Fe-Phen complex had a large oscillator strength value, which showed transient strength electron n to π* (Table 7) due to chromophore and auxochrome in the ligand (22).

The spectra results on ZINDO/s show the wavelength at Ni-Phen and Zn-Phen complex to change the transition from n to π* and π to π*. The results of this electronic transition calculation see how to translate electrons from HOMO to LUMO with different energy levels. Complex molecules that experience excitation with greater energy absorb light at shorter wavelengths. Conversely, molecules that experience excitation with less energy will absorb light at longer wavelengths. Modeling results, the electron transition for the Ni-Phen and Zn-Phen complex requires more energy to experience the electron transition from HOMO-2 to LUMO+2 which is characterized by peak absorption at short wavelengths in the transition type π to π*. In contrast, the electron transition from the Ni-Phen and Zn-Phen complex requires less energy to experience the electron transition from HOMO to LUMO which is characterized by absorption of peaks at long wavelengths in transition types n to π* (Tables 8 and tables 9).

Analysis of Spectra and Electronic Transitions

The determination of complex spectra was done by UV-Vis spectrophotometry and computation were done using method of semi-empirical ZINDO/s. The calculation result using ZINDO/s method is presented in the form of discontinuous spectrum modeling simulation. The result of calculation of electronic transition spectrum is obtained from electron transition process at the level of molecular orbitals, ie HOMO and LUMO complex ion Fe(III), Ni(II), and Zn(II) with complexing 1,10-phenanthroline.

Table 5: Results of Spectral Measurements of Spectra by UV-Vis Spectrophotometry

Complex	λ(nm)	Abs.
Fe-Phen	484.00	0.016
	364.00	0.185
	315.50	1.227
	469.00	0.016
	325.50	0.084
Ni-Phen	366.00	0.021
	343.50	0.069
	325.00	0.219
	355.00	0.017
	336.50	0.027
Zn-Phen	315.00	1.704

The load values for the Fe-Phen, Ni-Phen, and Zn-Phen complexes have been calculated using the PM3 and ZINDO/s methods. The charge price shows the tendency of the distribution of electrons in the bonds that occur between metal ions (Fe(III), Ni(II), and Zn(II)) with 1,10-phenanthroline. These electron distributions help indicate how much the coordination covalent bond strengths in the three complexes (27).

Table 6: Comparison of Fe-Phen Complex Charge (eV) Using PM3 and ZINDO/s Methods.

Atom	PM3	ZINDO/s
N_{5}'	0.458976	-0.187097
N_{11}'	0.403515	-0.219591
N_{19}'	0.368995	-0.214342
N_{25}'	0.368761	-0.214750
N_{33}'	0.459333	-0.187022
N_{39}'	0.401748	-0.219964
Fe_{43}'	-0.616334	0.118759

Generally, the total value of charge on each atom shows the identity of the charge on a complex molecule. The charge ratio for the Fe-Phen complex using the PM3 and ZINDO/s methods shows the different results in the atoms involved in the coordination covalent bonds (Tabel 6). In addition, experimental spectral measurements have been made using UV-Vis spectrophotometers and electronic transition simulations using ZINDO/s. The measured wavelength in the Fe-Phen complex, ie 315.50 nm with an absorbance value of 1.227 (Table 5). Meanwhile, for ZINDO/s method results obtained wavelength with the number of 18 transitions. The wavelength with the highest peak measured lies at 437.36 nm (f: 0.249), 317.47 nm (f: 0.265) and 305.48 nm (f: 0.521) indicating the electron n transfer to π* (Table 7).

Table 7: Computational Results of Fe-Phen Complex Using Semi-Empirical Method ZINDO/s

λ(nm)	Osc. (f)	Transition
437.36	0.249	$n \rightarrow \pi^*$
317.47	0.265	$n \rightarrow \pi^*$
305.48	0.521	$n \rightarrow \pi^*$

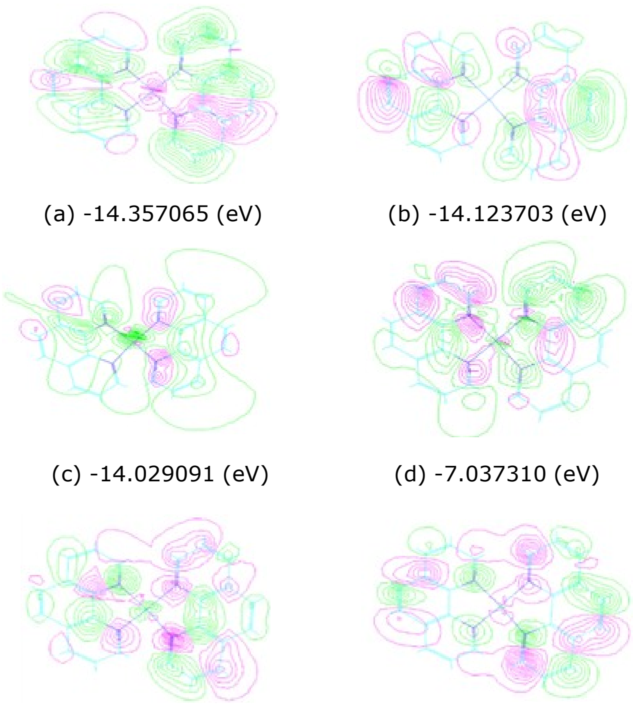
The calculation of the electron transition simulation in the Fe-Phen complex involves 67 atoms and 201 orbitals from HOMO to LUMO can not be selected using the ZINDO/s method. The reason was optimization of geometry (PM3) with a 0.01 kcal/Å.mol gradient was not capable of simulating geometry calculations that have minimum energy based on half electron orbital filling approach, consequently calculations using ZINDO/s especially on electron transition energy from orbital (HOMO- LUMO) Fe-Phen complex is not readable on its calculated output. The peak with a large oscillator strength taken in the ZINDO/s simulation was expected to be measured at that wavelength by UV-Vis spectrophotometer experiments. Some small oscillator strength may not appear or be measured experimentally at these wavelengths (22, 28).

Table 8: Computational Results of Ni-Phen Complex Using Semi-Empirical Method ZINDO/s.

λ(nm)	Osc. (f)	MO level	DE (eV)	Transition
325.73	0.239	70→71	6.71	n→π*
		69→72	7.31	
283.26	0.133	68→71	7.31	n→π*
272.85	0.054	68→72	7.55	n→π*
258.46	0.102	69→73	7.57	n→π*
254.51	0.085	70→71	6.71	n→π*
		69→72	7.31	
253.35	1.208	70→73	7.48	n→π*
244.44	0.855	68→73	7.80	π→π*

The measured spectra of the UV-Vis spectrophotometer showed the greatest absorbance, ie 0.219 at the 325 nm wavelength for the Ni-Phen complex (Table 5). The spectral results in ZINDO/s show the wavelength with 7 peaks. One of the measured peaks in the absorbance near the experimental value is at the wavelength 325.73 (f: 0.239) which shows the electronic transition n to π* (Table 8). This is due to the presence of benzene ring chromophores and amide groups in ligands 1,10-phenanthroline so that the measured wavelength range is in the UV region.

Semi-empirical ZINDO/s modeling method on the Ni-Phen complex involves 45 atoms and 137 orbitals. Energy changes in each molecular orbitals of Ni-Phen complex shift from HOMO to LUMO. The levels of molecular orbital 68 (HOMO-2 / π3), 69 (HOMO-1 / π2) and 70 (HOMO / π1), the molecular orbital level 71 (LUMO / π-1), 72 (LUMO +\1 / π-2) and 73 (LUMO +2 / π-3) (29, 30). The energy differences of the gap (DE) influenced the electron for excitation from HOMO to LUMO. The lower energy differences of a molecule, the easier it will be to excel from HOMO to LUMO, as in Ni-Phen complex, there's a shift from the 70 to 71 orbital which is the largest electron transition and the 68 to 73 orbital which is the smallest electron transition. The energy level of HOMO-LUMO of complex Fe-Phen, Ni-Phen, and Zn-Phen was shown in Figure 3.



(a) -14.357065 (eV)

(b) -14.123703 (eV)

(c) -14.029091 (eV)

(d) -7.037310 (eV)

(e) -6.805417 (eV)

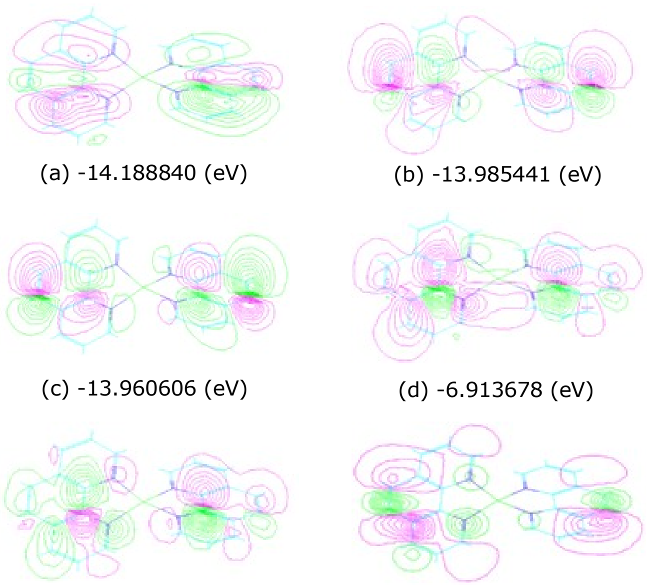
(f) -6.547492 (eV)

Figure 3. Levels of Complex OM Ni-Phen (a), (b), (c) HOMO 68, 69, 70 and (d), (e), (f) LUMO 71.72, 73.

The measured Zn-Phen spectra on the UV-Vis spectrophotometer were at a wavelength of 315 nm with an absorbance of 1.704 (Table 5). Computational determination of the spectra has also been performed using the ZINDO/s method by showing 6 different transitions of intensity (Osc). The transition of electrons to the Zn-Phen complex involves 55 atoms and 132 orbitals, shifting the degree of complex molecular orbitals leading to changes in energy. Where some of the peaks that arise may not be like the data obtained experimentally. One of the peaks approaching the experimental result is 325.91 nm (f: 0.334) with n electron transition to π* (Table 9).

Table 9. Computational Results of Zn-Phen Complex Using Semi-Empirical Method ZINDO/s.

λ(nm)	Osc (f)	MO Level	DE (eV)	Transition
325.91	0.334	64→67	7.27	$n\rightarrow\pi^*$
		64→68	7.32	
289.79	0.568	64→67	7.27	$n\rightarrow\pi^*$
		64→68	7.32	
261.97	0.050	64→67	7.27	$n\rightarrow\pi^*$
		64→68	7.32	
246.24	0.682	66→69	7.81	$\pi\rightarrow\pi^*$
		65→69	7.84	
230.15	0.380	66→69	7.81	$\pi\rightarrow\pi^*$
		65→69	7.84	
226.20	0.714	64→69	8.04	$\pi\rightarrow\pi^*$



(a) -14.188840 (eV)

(b) -13.985441 (eV)

(c) -13.960606 (eV)

(d) -6.913678 (eV)

(e) -6.861319 (eV)

(f) -6.141289 (eV)

Figure 4. Levels of Complex OM Zn-Phen (a), (b), (c) HOMO 64, 65, 66 and (d), (e), (f) LUMO 67, 68, 69.

The electron transition energy in the Zn-Phen orbital molecule of the complex can be observed in the energy changes of each molecular orbital (Figure 4). The occurrence of electronic transition from the HOMO orbital level to the LUMO was due to the free electron pair in the ligand 1,10-phenanthroline, consequently the optimum wavelength shift in the larger complex compound.

CONCLUSION

Optimization of complex molecular geometry using PM3 shows the results of total energy and different forms of geometry. The total energy for the Fe-Phen complex is -185756 (kcal / mol) (octahedral), the Ni-Phen complex was -135552 (kcal/mol) (planar quadrilateral) and Zn-Phen complex of -113570 (kcal/mol) (tetrahedral). Spectrophotometric UV-Vis spectrometric spectra measurements were measured at the highest absorbance with wavelength for Fe-Phen complex of 315.50 nm (1.227), Ni-Phen complex of 325.00 nm (0.017), and Zn-Phen complex of 315.00 nm (1.704). The electronic transition of complex molecules is carried out using the ZINDO/s semi-empirical method by reviewing some of the peaks that appear on the discontinuous spectrum and energy in the HOMO-LUMO molecular orbital. The transition type for the three complexes was in the transition range n to π* and π to π*.

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