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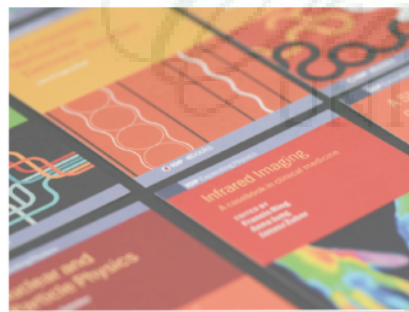
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Study of thermodynamics and complex structures on spin transitions of $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ and $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complexes using the Density Functional Theory method

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Abstract. The complex of iron(II) 1,2,4 H-triazole chloride is a complex that has spin transition characteristics. Thermodynamic studies and determination of changes in complex structured data have been carried out on the $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ and $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complexes with the DFT method. The iron(II) 1,2,4 H-triazole chloride complex has a polymeric structure, so in this study used a model with 2 and 4 Fe(II) ions. The computational chemistry study using a hybrid functional/basis set B3LYP/6-31G(d) results obtained show the distance between the Fe(II) ions, the bond length of Fe-N, and the distance between the Fe(II) ions with Cl⁻ in the $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex at low spin states respectively 3.717Å, 1.990Å-2.049Å, and 6.829Å, while in the high spin state respectively 3.932Å, 2.130Å-2.360Å and 7.050Å. The distance between the Fe(II) ions, the bond length of Fe-N, and the distance between the Fe(II) ions with Cl⁻ in the $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complex at low spin states respectively 3.661Å-3.681Å, 1.960Å-2.089Å and 5.037Å, while in the high spin state respectively 3.911Å-3.946Å, 2.092Å-2.367Å and 5.280Å. Thermodynamic data in $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex is $\Delta E=-24.38989\text{kJ/Mol}$, $\Delta H=-24.3909\text{kJ/Mol}$, $\Delta G=-47.9364\text{kJ/mol}$, and $\Delta S=0.0789\text{kJ/Mol}$. Thermodynamic data of $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complex is $\Delta E=-12.8564\text{kJ/Mol}$, $\Delta H=-12.8564\text{kJ/Mol}$, $\Delta G=-33.6445\text{kJ/Mol}$, and $\Delta S=0.0697\text{kJ/Mol}$. The structure and thermodynamic data are compatible with experimental measurement data in the laboratory.

Key words: thermodynamic data, complex structures, spin transitions, $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$, $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$, and DFT.

1. Introduction

The iron(II) 1,2,4 H-triazole complex is a complex that has a spin transition (TS). The characteristics of TS are the characteristics of compounds which are in the two states of the spin metal ion Fe(II) due to the influence of temperature, pressure, and light radiation. It has occurred due to ligands 1,2,4 H-triazole are ligands with medium ligand field strength. The ligands with the medium ligand field strength resulting in energy differences in low spin and high spin states that are very small, so that external influences will cause changes in the spin state of this complex compounds.

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Study of the iron(II) 1,2,4 H-triazole complex with various anions has been carried out by several previous researchers. Study of the $\text{Fe}(\text{trzH})_2(\text{trz})\text{X}$, with $\text{X} = \text{BF}_4^-$, ClO_4^- , and PF_6^- by measuring magnetism and the Mössbauer spectra. The results obtained show Fe(II) 1,2,4 H-triazole complex with BF_4^- and ClO_4^- anions have a transition temperature above room temperature, whereas for PF_6^- anions occur below room temperature [1]. A study on the properties of the iron(II) 1,2,4 H-triazole chloride complex shows the presence of the number of water molecules in the $[\text{Fe}(\text{Htrz})_3]\text{Cl}_2$ complex will shift the transition temperature to a lower temperature [2]. Faulmann, et al. [3] have succeeded in getting nano-sized complex $[\text{Fe}(\text{trz})_2(\text{trz})](\text{BF}_4)$ using silica matrices and reporting their transition temperatures above 100°C . In this study, we study the effect of changes in the spin state of Fe(II) ion on thermodynamic variables and complex structured data using computational chemistry methods. Changes in the spin state of the Fe(II) ion in the iron(II) 1,2,4 H-triazole chloride complex cause changes in thermodynamic variables and structural changes in this complex. The thermodynamic variables observed were Energy (E), Enthalpy (H), Gibbs free energy (G), and Entropy (S). Structure variables of iron(II) 1,2,4 H-triazole chloride complex observed the distance between Fe(II) ions, the bond length of Fe-N, and the distance between Fe(II) cations and Cl^- anions.

The computational studies on TS complex compounds have been carried out by several previous researchers. Study of complexes with Htrz derivatives, which are one-core complex with three ligands $[\text{Fe}(\text{Rdpt})_3](\text{BF}_4)$. In this study, eight types of ligands with different substrates on N^+ atoms observed, the results obtained were only one that is a spin transition (TS), which is complex $[\text{Fe}(\text{pldpt})_3](\text{BF}_4)_2 \cdot 1\frac{1}{2}\text{H}_2\text{O}$ [4]. The vibrational properties of $[\text{Fe}_3(4-(2\text{-hidroksi-etil})-1,2,4\text{-triazol})_6](\text{CF}_3\text{SO}_3)_6$ complex, which is a three-core complex has been studied using a nuclear inelastic scattering of synchrotron radiation (NIS). The results show the complex formed has TS properties in the Fe(II) ion with the FeN_6 framework while in the terminal section it has a FeN_3O_3 framework that does not exhibit TS properties [5]. The complex with two types of ligands namely stirilpyridine and NCX ($\text{X} = \text{S}, \text{Se}, \text{and BH}_3$) which are single-core complexes with the formula $[\text{Fe}(\text{stpy})_4(\text{NCX})_2]$ have been studied using computational chemistry methods [6]. The computational study determined the stability and structure of $[\text{Fe}_4(\text{Htrz})_8(\text{trz})_4]^{4+}$ and $[\text{Fe}_4(\text{Htrz})_{12}]^{8+}$ complexes. This study used the UHF, B3LYP, and TPSSH methods on a set basis of 3-21G, 6-31G (d), and TZVP. The results obtained show the complex $[\text{Fe}_4(\text{Htrz})_8(\text{trz})_4]^{4+}$ is more stable than the complex $[\text{Fe}_4(\text{Htrz})_{12}]^{8+}$ [7]. The other study of the structure parameters of Fe(II)-Htrz complex predicts the molecular formulas of Fe(II)-Htrz complex is $[\text{Fe}(\text{Htrz})_2\text{trz}]_n^+$ [8].

In this study, computational calculations use the DFT method with the B3LYP hybrid functional. There are several advantages and disadvantages of DFT compared to the HF theory approach. In some calculation cases, the HF theory is quite useful in determining the optimum structure. It is not right in determining the amount of energy while the DFT method is better for determining the amount of energy. In Hartree-Fock theory, multi-electron wave functions expressed with the Slater determinant which is built from a set of N single-electron wave functions. As in the Hartree-Fock theory on DFT also uses a single wave function. However, the Hartree-Fock theory calculates all N electron wave functions while DFT only calculates the total electron energy globally and the electron density distribution. Fock proposed the addition of Hartree SCF with the Determinant Slater wave function. Furthermore, Hartree Product orbitals, Hartree Fock (HF) molecular orbitals can be determined individually as eigenfunctions of a set of operators for one electron but now the interaction of each electron with the static field of all other electrons. The Fock operator for one electron defined for each electron i expressed in Equation 1. Fock proposed the addition of Hartree SCF with the Determinant Slater wave function. Furthermore Hartree Product orbitals, Hartree Fock (HF) molecular orbitals can be determined individually as eigenfunctions of a set of operators for one electron but now the interaction of each electron with the static field of all other electrons. The Fock operator for one electron is defined for each electron i expressed in Equation 1.

$$f_i = -\frac{1}{2}\nabla_i^2 - \sum_k \frac{Z_k}{r_{ik}} + V_i^{\text{HF}}\{j\} \quad (1)$$

The main idea of DFT the total electronic energy and distribution of electron densities globally. The Hohenberg-Kohn theorem shows the Thomas-Fermi model used as an approximation of the density

functional theory (DFT). In the DFT the total electronic energy function written as a function of electron density expressed in Equation 2.

$$E_{10} = E_{EK}(\rho) + E_c(\rho) + E_H(\rho) + E_{xc}(\rho) \quad (2)$$

Where: $E_{EK}(\rho)$ is kinetic energy, $E_c(\rho)$ is the interaction energy between nuclei, $E_H(\rho)$ is the electron-electron interaction energy and $E_{xc}(\rho)$ contains changes and contribution correlations. The interaction of all electrons contained in $E_H(\rho)$ and $E_{xc}(\rho)$. The conclusion obtained from the Hohenberg-Kohn theorem is the properties of the system in the ground state determined by the density. Improper density gives greater energy than actual energy. It is necessary to write variations of components in equation 2 in the density function and then optimize energy as the density function. The components that contribute to the energy in the first 2 part equation of the density function expressed in Equation 3.

$$E(\rho) = 2 \sum \int \psi_i \left(-\frac{\nabla^2}{2} \right) \psi_i dv + \int r_{nuclear} \rho(r) dv + \frac{1}{2} \iint dv dv' \frac{\rho(r)\rho(r')}{|r-r'|} + E_{xc}[\rho(r)] \quad (3)$$

For the term correlation balancer $E_{xc}[\rho(r)]$ several approximations must be made. The most common way to obtain this contribution is to use local density approximation based on uniform electron gas. If E_{xc} is the correlation correction energy per particle in a uniform electron gas then the total correlation balancing energy E_{xc} of the system can be obtained from the results of the integration presented in Equation 4.

$$E_{xc}[\rho(r)] \cong \int \rho(r) \varepsilon_{xc}[\rho(r)] dr \quad (4)$$

This result can be applied when the number of spins up is equal to the number of spins down and cannot be applied to systems with an odd number of electrons in calculating the density function, energy optimized by being dependent on density. Usually the use of Kohn and Sham densities is applied to derive from the Slater determinants with orthonormal orbitals. Using Kohn-Sham orbitals allows energy for optimization through solving a set of one electron equations but using electron correlations. It is one of the critical advantages of the density function approach. The Kohn-Sham equation stated in Equation 5.

$$\left[-\frac{\nabla^2}{2} + r_{nuclear}(r) + \int dv' \frac{\rho(r')}{|r-r'|} + r_{xc}(r) \right] \psi_i(r) = \varepsilon_i \psi_i(r) \quad (5)$$

$r_{xc}(r)$ can be obtained easily from an exact analytic statement of the local density approximation [9].

The B3LYP hybrid functional has been used to determine the structure, energy, vibration spectra, and spin transitions. Structural studies using the DFT method with the B3LYP hybrid function have been carried out on 13 types of compounds [10] and 4-amino-1,2,4-triazole compounds [11]. The results of the calculation of heat formation using the B3LYP method against 49 tetrazole-derived compounds, obtained there are 5 compounds of difference values with experiments smaller than 2 kJ/Mol [12]. Study of the structure and energy of 15 N2CP isomers [13], triphenylamine [14], and 3-Phenylamino-4-Phenyl-1,2,4-Triazole-5-Thione compounds [15]. The effect of adding triple-basis 6-311G basis sets on the calculation of vibrational frequencies from the combination of diffuse and function [16] and the determination of vibration spectra using B3LYP and OLYP with base sets 6-31G(d) [17]. Calculations using B3LYP/ 3-21G(*) and PBEPBE/ 6-31G (d) used for structural prediction. A spectroscopic data from porphyrin-quinone, porphyrin-hydroquinone, supramolecules porphyrin-quinone dyads and porphyrin hetero dimers [18]. Study of transition spin and thermal hysteresis at $[\text{Fe}(\text{Htrz})_2(\text{trz})](\text{BF}_4)$ and $[\text{Fe}(\text{Htrz})_3](\text{BF}_4)_2 \cdot \text{H}_2\text{O}$ (Htrz = 1,2,4-4H-triazole; trz = 1,2,4-triazolato [19]. The study of transition spin with B3LYP double- ζ basis set in the complex $[\text{Fe}(\text{DAPP})(\text{abpt})](\text{ClO}_4)_2$ shows the percent error for bond lengths and bond angles at HS states respectively by 2,033% and 0,901% and the LS situation about 2,369% and 0,930% [20].

The B3LYP method is a method of Density Functional Theory (DFT) using the electron density function. The electron density $\rho(\vec{r})$ defined as the multiple integral spin coordinates of all electrons given in Equation 6.

$$\rho(\vec{r}) = N \int \dots \int |\psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N)|^2 ds_1 d\vec{x}_2 \dots d\vec{x}_N \quad (6)$$

$\rho(\vec{r})$ determine the probability of finding N electrons in the volume of $d\vec{r}$, $\rho(r)$ is the probability of density.

Kohn and Sham proposed the separation of the density function F [ρ] in equation 7.

$$F[\rho(\vec{r})] = J[\rho(\vec{r})] + E_{xc}[\rho(\vec{r})] \quad (7)$$

where E_{xc} , called exchange-correlation energy, is defined in equation 8

$$E_{XC}[\rho] \equiv T[\rho] - T_s[\rho] + (E_{ee}[\rho] - J[\rho]) = T_C[\rho] + E_{ncl}[\rho] \quad (8)$$

Becke, 1993b introduces semiempirical coefficients to determine the weights of the components given in equation 9.

$$E_{XC}^{B3} = E_{XC}^{LSD} + a(E_{XC}^{\chi=0} - E_{XC}^{LSD}) + bE_X^B + cE_C^{PW91} \quad (9)$$

Equation 4 has three parameters, the value of the function change is determined by a, while b and c are controls of the change in contribution and correction of the correlation gradient for the local density approximation.

Furthermore, the most popular hybrid function is B3LYP and suggested by Stephens et al. [21]. The value of the three parameters has been stated in Becke's original paper. The statement of changes in the B3LYP correlation energy is given in equation 10.

$$E_{XC}^{B3LYP} = (1 - a)E_X^{LSD} + aE_X^{\chi=0} + bE_X^{B88} + cE_C^{LYP} + (1 - c)E_C^{LSD} \quad (10)$$

[22]

2. Computational Method

Computational chemistry studies are studies in determining the properties of compounds using quantum chemical calculations. In computational chemistry calculations, the geometry optimized for the "trial and error" structure and the amount of energy of the structure determined. Geometry optimization is a way to determine the lowest energy using a certain basis set (molecular orbitals provided).

The computational chemistry calculations using Gaussian 09 Revision D.01 software [23] and visualization of calculation results using Jmol software [24]. The method used in computational chemistry calculations is the Density Functional Theory (DFT) method with the B3LYP hybrid functional, while the basis set used 6-31G(d). The complex compounds observed in this study have a polymeric structure so that in computational chemistry calculations structural modelling performed. The model used is to use 2 Fe(II) ions with nine ligand rings 1,2,4 H-triazole and one of Cl⁻ ion and 4 Fe(II) ions with 15 ligand rings and three of Cl⁻ ions.

3. Results and Discussion

The discussion in this study grouped into three parts, namely: the structure of computer simulation results, structure data, thermodynamic variable data from the iron(II) 1,2,4 H-triazole chloride complex in the low spin state and high spin state.

3.1. The structure of the iron(II) 1,2,4 H-triazole chloride complex in the low spin and high spin states. The computational chemistry calculation results visualized using Jmol software, so that the complex structure of [Fe₂(Htrz)₆(trz)₃]Cl is obtained in the low spin state and high spin state. Visually, the complex structure resulting from computational chemistry calculations at low spin states does not differ from structures at high spin states. The complex structure of [Fe₂(Htrz)₆(trz)₃]Cl visualization results with Jmol software are presented in Figure 1.



Figure 1. Structure of visualization results of [Fe₂(Htrz)₆(trz)₃]Cl complex results of calculations on the hybrid functional/ basis set B3LYP/ 6-31G(d) in the (a) low spin and (b) high spin states

The structure of the visualization results of the $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complex for the calculation results on the hybrid functional/ basis set B3LYP/ 6-31G(d) in the low spin and high spin states shown in Figure 2.

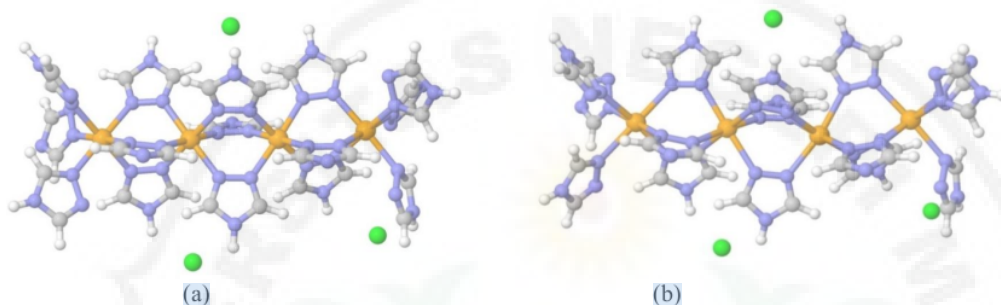


Figure 2. Structure of visualization results of complex $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ results of calculations on the hybrid functional/ basis set B3LYP/ 6-31G(d) in (a) low spin and (b) high spin states.

3.2. Data on the structure of iron(II) 1,2,4 H-triazole chloride complex at low spin and high spin.

Visually, the complex structure in the low spin and high spin states is similar, but based on the data the structure of the value is different. Based on the visualization results on the $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex, the distance between Fe(II) ions in the low spin state is 3.717Å and in the high spin state is 3.932Å. The bond length of the Fe-N in the low spin state is 1.990Å – 2.049Å and the high spin state is 2.130Å – 2.360Å. The distance between the Fe(II) ion and the Cl⁻ ion at a low spin state is 6.829Å and a high spin state is 7.050Å. The results of experimental measurements of the $[\text{Fe}(\text{Htrz})_2(\text{trz})]\text{BF}_4$ complex show the distance between Fe(II) ions in the low spin state is 3.671(1)Å and in the high spin state is 3.891(1)Å, while the bond length of the Fe-N in the low spin state is 1.827(5)Å – 1.981(6)Å and the high spin state is 2.040(2)Å-2.042(5)Å [25]. This data shows the distance between Fe(II) ions and the bond length of Fe-N calculated by computational chemistry by the experimental results. Based on these data, it obtained the structured data at the low spin state are smaller than the high spin state. Data on the distance between the Fe(II) ions, the bond length of Fe-N, and the distance between the Fe(II) ions and the Cl⁻ ions from the computational chemistry calculations using the hybrid functional/ basis set B3LYP/ 6-31G(d) on the $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex are presented in Table 1.

Table 1. The distance between Fe(II) ions, the bond length of Fe-N, and distance between Fe(II) and Cl⁻ in the $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex using the hybrid functional/ basis set B3LYP/ 6-31G(d).

Spin state	Low Spin	High Spin
The distance between of Fe(II) ion (Å)	3.717	3.932
The bond length of Fe-N (Å)	1.990 – 2.049	2.130 – 2.360
The distance between of Fe(II) ion with Cl ⁻ ion (Å)	6.829	7.050

Based on the results of visualization on the $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complex, it found that the distance between Fe(II) ions in the low spin state is 3.661 – 3.681Å and in the high spin state is 3.911 – 3.946Å. The bond length of the Fe-N in the low spin state is 1.960 – 2.089Å and in the high spin state is 2.092 – 2.367Å. The distance between the Fe(II) ion and the Cl⁻ ion in the low spin state is 6.037Å and in the high spin state is 5.280Å. Based on these data, it obtained the structured data at the low spin state are smaller than at the high spin state. They are changing the spin state of Fe (II) from a low spin state to a high spin state that increases in bond lengths and distances between atoms. Data on the distance between the Fe(II) ions, the bond length of the Fe-N, and the distance between the Fe(II) ions and the Cl⁻ ions from the computational chemical calculations using the hybrid functional/ basis set B3LYP/ 6-31G(d) on the complex $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ presented in Table 2.

Table 2. The distance between Fe(II) ions, the bond length of Fe-N, and distance between Fe(II) and Cl in the $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complex using the hybrid functional/ basis set B3LYP/ 6- 31G(d).

Spin state	Low Spin	High Spin
The distance between of Fe(II) ion (Å)	3.661 – 3.681	3.911 – 3.946
The bond length of Fe-N (Å)	1.960 – 2.089	2.092 – 2.367
The distance between of Fe(II) ion with Cl ion (Å)	5.037	5.280

3.3. Thermodynamic variables of the iron (II) 1,2,4 H-triazole chloride complex in the low spin and high spin states.

The changes in the spin state of Fe(II) ion also result in changes in chemical thermodynamic variables. Thermodynamic complex data of $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex has a value of $\Delta E = -24,38896\text{kJ/ Mol}$, $\Delta H = -24.3909\text{kJ/ Mol}$, $\Delta G = -47.9364\text{kJ/ Mol}$, and $\Delta S = 0.0789\text{kJ/ Mol.K}$. The data obtained from computational chemistry calculations are in accordance with the experimental measurement data. The experimental results of complex $[\text{Fe}(\text{Htrz})_2(\text{trz})](\text{BF}_4)$ measurements for ΔH_{TS} were 27.8 kJ/ Mol [19] and ΔS_{TS} were 0.075 kJ/ Mol.K [26]. Data E, H, G, and S computational results using the B3LYP hybrid function and base set 6-31G(d) in the $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex is presented in Table 3.

Table 3. Thermodynamic data calculation results on the $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex

No	Thermodynamic Variable	Energy (Ht)			The change of Energy (kJ/mol)	(The change of Energy)/n (kJ/mol)
		Low Spin State	High Spin state	The Difference		
1	E	-5165.5646	-5165.5832	-0.018579	-48.7792	-24.3896
2	H	-5165.5637	-5165.5823	-0.01858	-48.7818	-24.3909
3	G	-5165.6903	-5165.7268	-0.036516	-95.8727	-47.9364
4	S (kal/mol.K)	266.425	304.177	37.752	0.1578	0.0789

Based on the results of computational chemistry calculations with the hybrid functional/ basis set B3LYP/ 6-31G(d) on the complex $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ obtained data of $\Delta E = -12.8564\text{kJ/ Mol}$, $\Delta H = -12.8564\text{kJ/ Mol}$, $\Delta G = -29.6445\text{kJ/ Mol}$, and $\Delta S = 0.0697\text{kJ/ Mol.K}$. The data of E, H, G, and S from computational results using the B3LYP hybrid functional and 6-31G(d) basis set in the $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complex is presented in Table 4.

Table 4. Thermodynamic data calculation results on the $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complex

No	Thermodynamic Variable	Energy (Ht)			The change of Energy (kJ/mol)	(The change of Energy)/n (kJ/mol)
		Low Spin State	High Spin state	The Difference		
1	E	-10065.4653	10065.4849	-0.01959	-51.4257	-12.8564
2	H	-10065.4644	10065.4840	-0.01959	-51.4257	-12.8564
3	G	-10065.6546	10065.7059	-0.05126	-134.5779	-33.6445
4	S (kal/mol.K)	400.472	467.129	66.657	0.2786	0.0697

4. Conclusion

Based on the visualization results on the $[\text{Fe}_2(\text{Htrz})_6(\text{trz})_3]\text{Cl}$ complex, the distance between Fe(II) ions in the low spin state is 3.717Å and in the high spin state is 3.932Å . The bond length of the Fe-N in the low spin state is $1.990\text{Å} - 2.049\text{Å}$ and in the high spin state is $2.130\text{Å} - 2.360\text{Å}$. The distance between the Fe(II) ion and the Cl ion at a low spin state is 6.829Å and at a high spin state is 7.050Å . The data obtained the $[\text{Fe}_4(\text{Htrz})_{10}(\text{trz})_5]\text{Cl}_3$ complex show the distance between Fe(II) ions in the low spin

state is 3.661 – 3.681Å and in the high spin state is 3.911 – 3.946Å. The bond length of Fe-N in the low spin state is 1.960 – 2.089Å and in the high spin state is 2.092 – 2.367Å. The distance between the Fe(II) ion and the Cl⁻ ion in the low spin state is 5.037Å and in the high spin state is 5.037Å. The data of $\Delta E = -24.3896 \text{ kJ/ Mol}$, $\Delta H = -24.3909 \text{ kJ/ Mol}$, $\Delta G = -47.9364 \text{ kJ/ Mol}$, and $\Delta S = 0.0789 \text{ kJ/ Mol}$. The thermodynamic function data by the experimental data.

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