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Computational Study of Fe(II) Complex Compound Structure Prediction with Thiocyanate (SCN^-) and Pyridin (C_5H_5N) Ligands Using the RHF (*Restricted Hartree Fock*) Method

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ABSTRACT

The formation of Fe(II) complex compounds with thiocyanate (SCN^-) as well as pyridin (C_5H_5N) forms a tetrapyridinditiocyanateobesi(II) complex compound, $[Fe(SCN)_2(py)_4]$. The comparison of these complex compounds is still engineering, so the researchers examined the comparison of the structure of stable complex compounds on Fe(II) with thiocyanate and pyridin ligands, by continuing previous research using computational chemistry. Complex compounds that are more stable and the most suitable molecular formula based on computational calculations using RHF hybrid functions and 6-31G basis sets, geometry optimization of molecules from NWChem version 6.6 and Jmol software version 14.28.29. The energy of the computational calculation using RHF/6-31G for the structure $Fe(SCN)_2(C_5H_5N)_4$: -1524.86976182444 KJ/mol; $Fe(SCN)_3(C_5H_5N)_3$ structure: -1557.98302881166 KJ/mol; and $Fe(SCN)_4(C_5H_5N)_2$ structure: -2083.53616162888 KJ/mol. The change in formation energy indicates that the structure of $Fe(SCN)_4(C_5H_5N)_2$ is the most stable. The most suitable molecular formula for the Fe(II) complex compound is $[Fe(SCN)_4(C_5H_5N)_2]$.

Keywords: Pyridine, thiocyanate, NWChem, chemistry computional

1. INTRODUCTION

In recent years, the use of Computational Chemistry is very frequent and has become widespread because it is very helpful in molecular modeling. In the process of Computational simulation, simplifications are made and can be considered as an easy way to visualize in connecting theory with experiment [12].

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Computational Chemistry applies the principles of theoretical Chemistry, supported by computer programs, to calculate energies and analyze properties and transformations of compounds. It is capable of simulating a wide range of molecules, from simple to highly complex structures. Molecular properties that can be calculated include atomic structure, energy values and differences, charge, dipole moment, reactivity, vibration frequency, and various spectroscopic parameters [8].

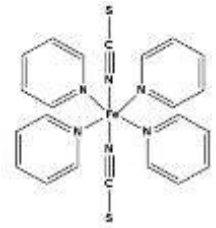
NWChem is a Computational software used in the fields of biomolecular chemistry, quantum chemistry. Classical chemistry, and others. Which will be run on a computer to analyze the data to be studied. This software will make the processed data into a stable structure. NWChem is also useful for inputting data from Avogadro *software* [1].

Avogadro is an advanced molecular editor and visualizer, molecular modeling, bioinformatics, materials science, and other related fields. It can be utilized by students for molecular visualization and three-dimensional molecular simulation; users can minimize their tertiary structure and view it from every possible angle and perspective [9].

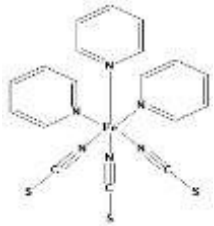
Fe(II) has an outer electron configuration of d^6. The electron configuration of Fe(II) can form complex compounds with different magnetic properties depending on the strength of the ligand field. The strong ligand field causes the Fe(II) complex to be diamagnetic because all the electrons are paired (low spin) while the weak ligand field is paramagnetic because there are four unpaired electrons (high spin [10].

The synthesis of the $[Fe(NCS)_6]^{4-}$ complex compound produced pale yellow paramagnetic crystals, while the $[Fe(NCS)_2(py)_4]$ complex produced dark purple diamagnetic crystals [2].

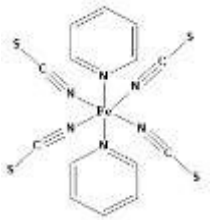
Fe(II) with pyridin and thiocyanate ligands can form the following complex compounds:



(a) $Fe(NCS)_2(py)_4$



(b) $Fe(NCS_{)3}(py)_3$



(c) $Fe(NCS)_4(py)_2$

In this study, computational chemistry calculations were carried out to determine the most likely correct structure which is the structure that has the smallest energy change.

Usually Fe(II) forms complex compounds with coordination numbers 4 and 6. Coordination number 4 is likely the geometric shape of the building tetrahedron and square and for coordination number 6 has a molecular geometry shape that is octahedral. And the formation of Fe(II) complex compounds with thiocyanate (SCN^-) as well as pyridin (C_5H_5N) forms a tetrapyridinditiocyanate-iron(II) complex compound, $[Fe(SCN)_2(py)_4]$. The comparison of these complex compounds is still engineering, so the researcher examines the comparison of the structure of stable complex compounds on Fe(II) with thiocyanate and pyridin ligands, therefore the author feels the need to continue previous research using computational chemistry.

2. EXPERIMENTAL

2.1.2 Research Tools

2.2.1 Hardware

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This research uses 2 computer devices with specifications:

- Processor type Intel Core™ i2-6100T CPU 3.20 GHz
- RAM (Random Acces Memory) 4.00 GB
- System type 64-bit Operating System Linux Ubuntu

2.2.2 Software

Geometry optimization of molecules from NWChem version 6.6 was carried out by ab initio method with RHF/6-31G basis set. Computational results were visualized using Jmol software version 14.28.29 for windows.

2.2. Research Procedure

1. Set up a computer by downloading Avogadro software to draw the structure to be studied.
2. Compiled NWChem data using notepad:
   a. Converted the structure into compact Z-Matrix data.
   b. Added commands for computational calculations such as charge, multiplicity, Basis Set, and calculation commands (RHF).
3. The file is saved with the namefile.nw1 and stored in one folder.
4. Perform computational calculations:
   a. Opened the terminal in Xubuntu.
   b. Created a calculation folder on each compound to be studied.
   c. Enter the calculation terminal.
   d. Written calculation command NWChem → file name.nw1 > file name.log&.
   e. Checked the calculation number and made sure the calculation was running.
   f. Pressed ctrl+shift and the
   g. The calculation number will disappear if the calculation has been completed.
   h. Check the calculation results by typing “less-nama file.log” then pressing enter.
   i. If the calculation is complete, “Optimization Converged” will appear along with the citation of the NWChem author and many files will appear in the compound folder that has been calculated.
   j. If there are none, information on the cause of the “error” is checked and the input data is corrected and recalculated by returning to step 3 part c.
   k. After success, search for the thermodynamic function in the.log file.
5. Create a visualization of the calculation results:
   a. Jmol software opened
   b. Open the.log file to obtain the structure of the resulting compound.
   c. When the structure is appropriate, the image is saved in JPG form.
6. Repeat the same steps for all compound structures to be calculated using NWChem

3. RESULTS AND DISCUSSION

3.1. Calculation Result Data

The results of computational chemistry with the RHF function and the 6-31G basis set are presented in Table 2.

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Table 1. Data from NWChem Calculation Results

	Energy (KJ/mol)
Fe	-1262.07621875
Pyridin	-246.59389820
Thiocyanate	32.76886075722
$Fe(SCN)_4(py)_2$	-3707.78385186
$Fe(SCN)_3(py)_3$	-3461.53435989
$Fe(SCN)_2(py)_3$	-3707.72473375

Table 2. ΔE data.

	Energy (KJ/mol)
$Fe(NCS)_4(py)_2$	-1524.86976182444
$Fe(NCS)_3(py)_3$	-1557.98302881166
$Fe(NCS)_2(py)_4$	-2083.53616162888

Based on Table 1 above, the data from computational chemistry calculations obtained the smaller $Fe(SCN)_4(py)_2$ structure with the smallest total energy. However, this data cannot be used to determine the stable structure. The most stable structure is determined by the value of the change in formation energy (ΔE).

In Table 2, an explanation can be obtained and it is known that the most stable structure is the structure with the lowest amount of change in formation energy. Based on the calculation results, the $Fe(NCS)_2(py)_4$ compound has an energy of -2083.53616162888 KJ/mol. When compared with $Fe(NCS)_3(py)_3$ and $Fe(NCS)_4(py)_2$ compounds, the energy of the $Fe(NCS)_2(py)_4$ complex compound is the lowest.

3.2 Visualization of Computation Result

The results of computational chemistry calculations using the RHF basis set 6-31G function obtained wave function data resulting from geometry optimization. These data can be visualized using Jmol software. The visualization results with Jmol are presented in Figure 1, Figure 2 and Figure 3.

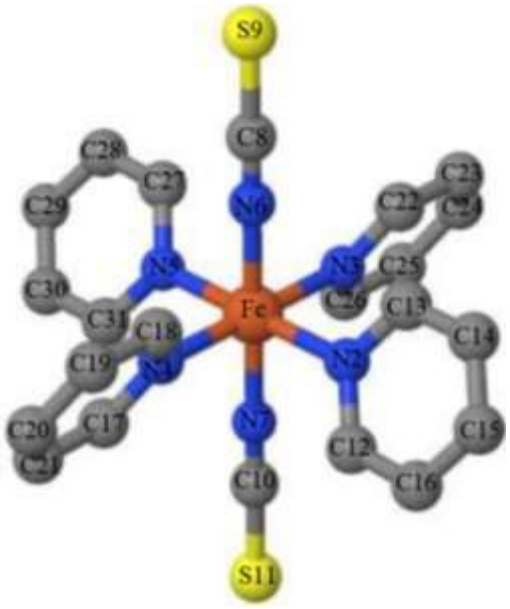

Figure 1. $Fe(NCS)_2(py)_4$ structure visualization results

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Based on figure 1, it can be seen that all pyridin ligands are in one plane with an angle of 90°and thiocyanate ligands are on the *y-axis* with an angle of 179.9°.

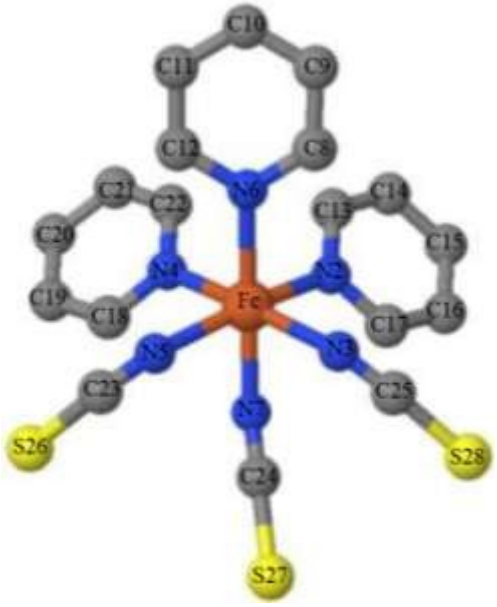

Figure 2. $Fe(NCS)_3(py)_3$ structure visualization results

Based on Figure 2, it can be seen that all pyridin ligands are in different planes with a large angle of 91.5° and thiocyanate ligands are also in different axes with a large angle of 90.0

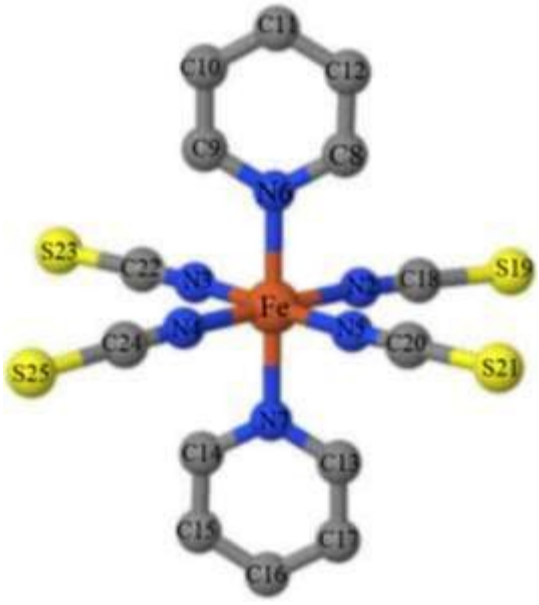

Figure 3. $Fe(NCS)_4(py)_2$ structure visualization results

Based on Figure 3, it can be seen that all pyridin ligands are in one plane with an angle of 179.8° and thiocyanate ligands are in the same plane with an angle of 89.9°.

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3.3 Bond Length Data of Compounds

Table 3. Bond length data of compounds visualized using Jmol software.

Structure	Bonding	(Å)
$Fe(NCS)_2(py)_4$	Fe-N6-7	1.95
	Fe-N2-5	2.02
$Fe(NCS)_3(py)_3$	Fe-N3,5,7	2.0
	Fe-N2,4,6	2.02
$Fe(NCS)_4(py)_2$	Fe-N6-7	2.01
	Fe-N2-5	1.95

According to Nugraha, et al (2022) that computational chemistry calculations use quantum chemical theory to determine the lowest energy (minimum energy) of a chemical structure. The minimum energy obtained is the energy of the most stable structure.

Bond length is inversely proportional to bond energy. The shorter the distance between atoms, the bond energy tends to be greater because the attractive force between atomic nuclei and electrons becomes stronger. Conversely, the longer the distance between atoms, the bond energy will decrease as the strength of the interaction decreases.

The stability of the complex compound is analyzed based on the total energy value. The lower the total energy, the more stable the complex compound. The complex with the configuration $[Fe(SCN)_4(C_5H_5N)_2]$ has the lowest total energy, which indicates that this compound is the most stable. This is due to the electron donor nature of SCN^- which is stronger than pyridin, thus increasing the interaction with the Fe(II) metal center.

Based on the calculation using RHF function and 6-31G basis set, the most stable molecular formula prediction is $[Fe(SCN)_4(C_5H_5N)_2]$.

4. CONCLUSION

The amount of energy from computational calculations using RHF/6-31G for the structure of $Fe(SCN)_2(C_5H_5N)_4$: -1524.86976182444 KJ/mol; $Fe(SCN)_3(C_5H_5N)_3$ structure: -1557.98302881166 KJ/mol; and $Fe(SCN)_2(C_5H_5N)_4$ structure: -2083.53616162888 KJ/mol. The change of formation energy shows that the structure of $[Fe(SCN)_4(C_5H_5N)_2]$ is the most stable. The most suitable molecular formula for the Fe(II) complex compound is $[Fe(SCN)_4(C_5H_5N)_2]$.

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