ASEC 2025 Conference

The 6th International Electronic Conference on Applied Sciences

09–11 December 2025 | Online

MDPI

Unveiling the electronic structure of coordination compounds: A density functional theory study

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INTRODUCTION & AIM

For decades, coordination compounds have strongly demonstrated their importance in many daily disciplines and industries. Their applications include catalysts, magnetic materials, porous materials, biomedical applications, drug delivery, etc. Coordination compounds are also highly present in stereochemistry as chiral luminescent materials, homochiral, chiral liquid crystals, enantioselective sensors, chiroptical switches, and magnetochiral compounds. For all these reasons and many more, tremendous effort has been devoted to the study of coordination compounds experimentally and theoretically. The development of new potential theoretical approaches has made it fruitful to study this kind of compounds. In this contribution, a theoretical DFT -based study is performed on some complexes of an organic ligand with different metal ions in order to reveal the energetics of such reactions. First of all, the electronic structure of the studied ligand as well as the formed complex was optimized at DFT//B3LYP/6-31G(d) level of theory. Then, using various approaches such as Fukui functions, and based on the obtained optimized structure of the studied complexes at the level of B3LYP/6-31G(d), the possible sites responsible for chelation with the metal ions were determined. Finally, the energetics based on thermodynamic quantities calculations, such as enthalpy, were also investigated in order to predict the stability and thermochemistry of the studied coordination compounds. It was found that the stability and the structure of the complexes not only depend on the ligand but also on the nature of the metal ion.

METHOD

The calculations of the reaction under study have been done at B3LYP/6-31G(d) using Gaussian 09 and GaussView suit of programs. Parr functions have calculated using the atomic spin density of Mulliken (ASD). Local electrophilicity and nucleophilicity have been calculated using the polar model of Domingo et al.

RESULTS & DISCUSSION

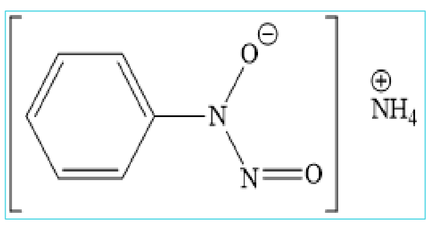

Figure 1: Structure of cupferron.

Table 1: Global properties of cupferron at B3LYP/6-31G(d).

	Cupferron				
E_{HOMO} (eV)	E_{LUMO} (eV)	μ(eV)	η(eV)	ω (eV)	N(eV)
0,24	3,41	1,82	1,59	1,05	0,35
	Cupferron ion				
-4,18	-0,45	-2,32	1,86	1,44	5,19

Cupferron has an electrophile index (ω = 1.05 eV) and a nucleophilicity of (N = 0.35 eV) and therefore is electrophilic.
The cupferron ion exhibits electrophilicity (ω = 1.44 eV) and nucleophilicity (N = 5.19 eV) and therefore is nucleophilic.

RESULTS & DISCUSSION

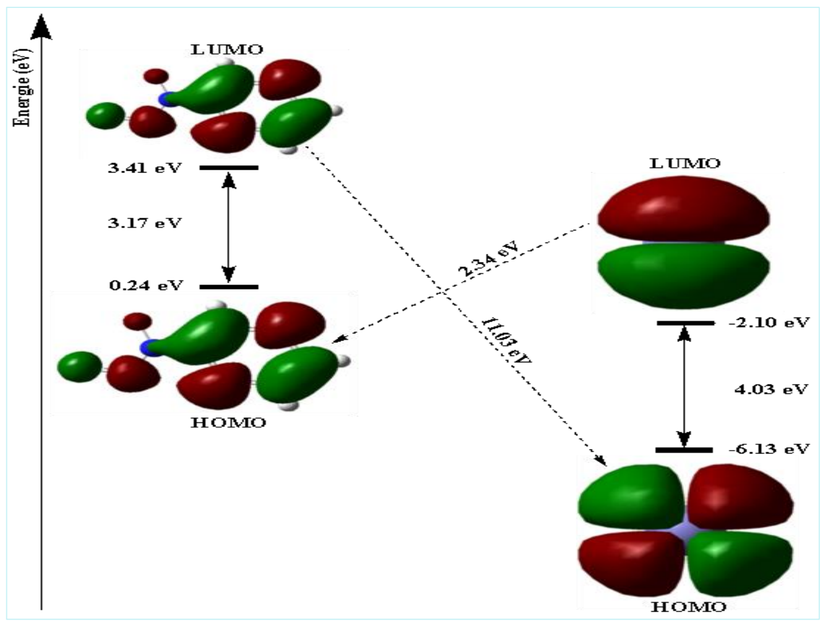

Figure 2: HOMO and LUMO interaction between cupferron and iron.

The gap $|HOMO_{cupferron} - LUMO_{metal\ ion}|$ is smaller in value than the gap $|HOMO_{metal\ ion} - LUMO_{cupferron}|$. This means that the formation of the corresponding complex studied will take place via this interaction.

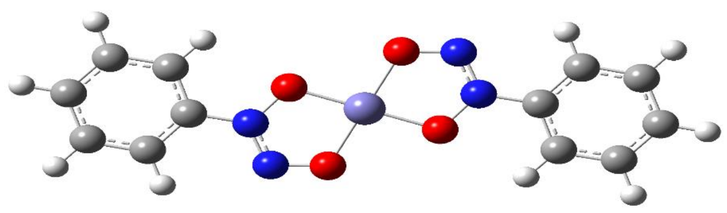

Figure 3: Optimized structure of the iron complex

CONCLUSION

The theoretical study has been done at B3LYP method in conjunction with 6-31G(d) basis set.

- The electrophilicity and nucleophilicity calculations show that cupferron is an electrophile while the corresponding ion is a nucleophiles.
- The possible interaction leading to the formation of iron complex with cupferron takes place between HOMO of cupferron and LUMO of iron ion with a gap of 2.34 eV.
- The obtained results show that the complex is formed in the presence of two ligands of cupferron to be linked to the iron ion Fe^{2+}.
- The structure of the obtained complex is a little bit twisted.

FUTURE WORK / REFERENCES

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3. Adhikari, S., Nath, S., Kansız, S., Balidya, N., Paul, A. K., Dege, N., ... & Safin, D. A. (2024). Zinc (II) coordination compound with N′-(pyridin-2-ylmethylene) nicotinohydrazide: Synthesis, crystal structure, computational and cytotoxicity studies. *Journal of Inorganic Biochemistry*, *257*, 112598.