22nd Iranian Inorganic Chemistry Conference,
23-25 August, 2023
University of Kurdistan

Electronic structure and properties of a new series of fac-Re(I) tricarbonyl complexes: a DFT study

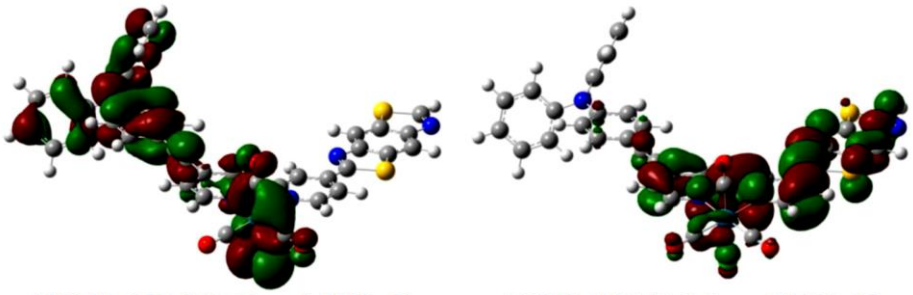
Akbar Bakhtiari [a] *

[a] *Department of Chemistry, Payame Noor University, 19395-4697, Tehran, Iran*

[*] *E-mail: akbar.bakhtiari@pnu.ac.ir*
bakhtiari.a1@gmail.com

Luminescence of rhenium(I) tricarbonyl diimine complexes was first reported by Wrighton and Morse in 1974 [1]. Since the first report, syntheses, photochemistry and photophysics of fac-[Re(Cl)(CO)$_3$(α-diimine)] complexes have been widely studied. These complexes have been reported as promising materials for potential applications in catalysis, sensors, organic light-emitting diodes, solar energy conversion, photosensitizers and possible agents in bioimaging and cancer therapy [2,3]. Structural modification of α-diimine ligand broadly affects the character and energy of HOMO and LUMO in these complexes [4]. Electron donor-acceptor (D-A) systems have been extensively investigated in recent years. To realize high performance photocatalysis in the multichromophore ensembles, controlling the charge transfer (CT) process is essential [5]. Depending on the energy levels of the metal and ligand orbitals, different excited states, including MLCT, LLCT, IL and SBLCT can be generated.

In this research work, electronic structure of four fac-[Re(Cl)(CO)$_3$(α-diimine)] complexes with electron acceptor-acceptor and donor-acceptor substituted α-diimine ligands are studied by DFT method. Benzothiazole derivatives (as electron acceptor) and triphenylamine groups (as electron donor) were introduced to the α-diimine core. The effect of donor and acceptor groups on the character and energy of HOMO and LUMO will be discussed in details. Moreover, TDDFT calculations results will be investigated to understand the electronic spectra and excited states of the complexes.



HOMO (MO 196) E = - 5.3938 eV LUMO (MO 196) E = - 2.9628 eV

Keywords: Rhenium(I), α-diimine ligands, electron donor-acceptor, electronic structure, DFT

References

[1] M. Wrighton and D. L. Morse, *J. Am. Chem. Soc.*, **1974**, 96, 998.
[2] L. D. Ramos, L. H. Macedo, N. R.S. Gobo, K. T. de Oliveira, G. Cerchiaro and K. Frin, *Dalton Trans.*, **2020**, 49, 16154.
[3] K. Choroba, A. Maroń, A. Świtlicka, A. Szłapa-Kula, M. Siwy, J. Grzelak S. Maćkowski, T. Pedzinski, E. Schab-Balcerzak and B. Machura, Dalton Trans., **2021**, 50, 3943.
[4] A. M. Maron, A. Szapa-Kula, M. Matussek, R. Kruszyski, M. Siwy, H. Janeczek, J. Grzelak, S. Mackowski, E. Schab-Balcerzak and B. Machura, *Dalton Trans.*, **2020**,49, 4441.
[5] E. J. Rohwer, Y. Geng, M. Akbarimoosavi, L. M. L. Daku, O. Aleveque, E. Levillain, J. Hauser, A. Cannizzo, R. Häner, S. Decurtins, R. J. Stanley, T. Feurer, S.-X. Liu, *Chem. Eur. J.* **2021**, *27*, 5399.