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Theoretical Study on the cooperativity/anticooperativity of metal–carbonyl and metal–dihydrogen bonds in some complexes of group 6 transition metals

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The aim of this project is to study the structure, interaction energy, stabilization energy, cooperative/anticooperative energy and the nature of the metal-ligand bond in some group 6 transition metal complexes containing dihydrogen and carbonyl ligands. For this project, some complexes with the general formula $[M(\eta^2\text{-}H_2)(CO)_4L]$ (M= Cr, Mo or W; L= SiO, PH_3, NO^+, N_2, NC^-, CS, CO, and CN^-) were selected [1-3]. It should be noted that, ligand L is in the cis or trans position to the dihydrogen ligand. To carry out this project, the initial structures of the above complexes were optimized by Gaussian09 computing software at the BP86 and B3LYP levels and using the def2-TZVPP basis set. Then, the values of total interaction and stabilization energies, cooperative energy and the length of M–(η^2-H_2), M−CO and M–L bonds in the optimized complexes were calculated and compared. Then, using NBO calculations, the amount of the natural charges of atoms, hybrid orbitals and bond orders were checked in each complex. Good correlations were observed, only in trans isomers, between the values of positive cooperative energies with the length and Wiberg bond order of the M–(η^2-H_2) bond. The lowest bond order and the longest M–(η^2-H_2) bond length were observed for the complexes that have the highest values of anticooperative energies between (η^2-H_2)–$M(CO)_4$ and $M(CO)_4$–L bonds. Also, in all the trans complexes, the nature of bonds was investigated by the Energy Decomposition Analysis (EDA) method.

Keywords: Theoretical Study, Dihydrogen complexes, Interaction and stabilization energies, NBO calculation, EDA analysis

References

[1] Kubas, J. *PNAS.*, **2007**, 104, 6901-6907.

[2] Salehzadeh, S., and Maleki, M. *J.Comput,.Chem.*, **2016,** 37, 2899-2807.

[3] Hokmi, S., Salehzadeh, S., and Gholiee, Y. *J. Comput. Chem.*, **2021,** 1, 1-10.