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Theoretical studies on the cooperative effects of π…M-X bonds in complexes [{μ_2-E_2(NHC(R)$_2$)$_2$}(MX)$_2$](E=B , Al; R=H, CH_3, SiH_3, Dipp, F, Cl, Br, Ph; M=Cu, Ag, Au; X=F, Cl, Br) containing E≡E fragment stabilized by *N*-heterocyclic carbene

Mahsa Safaei [a] **and Mehdi Bayat***

* *E-mail: mehdi806@gmail.com*

Transition metal (TM)-alkyne π complexes are key compounds in organic synthesis and catalysis [1]. Such complexes form during catalytic processes and are important intermediates in many metal-catalyzed reactions in inorganic chemistry [2]. The structure optimization of the complexes has been done at the M05/def2-SVP level of theory, and the bond analysis and related structural investigations have been done at the M05/def2-TZVP level of theory. This study contains theoretical studies on the three metal complex structure, silver, gold and copper with triple bond B_2 and Al_2 stabilized by NHC ligands. Changing The structural characteristics of the complex will be reviewed when the R group attached to the NHC ligands and the halogen group attached to the metal are changed. Also, the cooperative effects of the bonds in the structure of this complex will be investigated. In all sections, different bonds have been investigated using Natural Bond Orbital (NBO), Energy Decomposition (EDA) and (ETS-NOCV) analyses.The stability energy of the complexes shows a better trend in the structures containing boron atom Based on the stability energy of the structures, the value of cooperativity (E_{Coop}) ($E_{COOP} = SE_{(ABC)} - SE_{(AB)} - SE_{(BC)}$, (AB) and (BC) fragments of (ABC), SE is stabilization energy) [3] was calculated for some B structures and the results showed that the investigated structures do not have cooperativity.

Keywords: NHC complexes, Cooperativity, (TM) alkyne π complexes , Boron-Boron multiple bonding

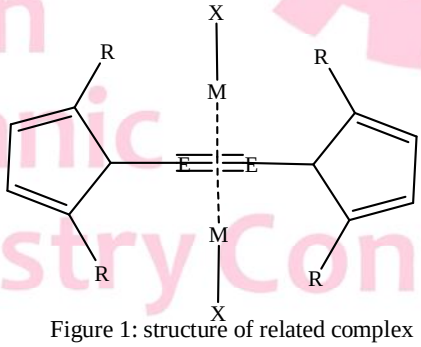


Figure 1: structure of related complex

E=B , Al
M=Cu, Ag and Au
X=F, Cl, Br
R=H, CH_3, SiH_3, Dipp, F, Cl, Br, Ph

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