

Theoretical studies on the nature of metal-ligand bonds in some cylinder-like trinuclear hexacarbene complexes of Cu(I), Ag(I), Au(I), Pd(II) and Hg(II) ions

Khadije naeemi^a and mehdi bayat^{*a}

^aDepartment of Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan, Iran

* E-mail: mehdi806@gmail.com

N-Heterocyclic carbenes (NHCs) have been extensively investigated over the last two decades due to their applications in various fields like as spectator ligands in catalytically active complexes, [1] in materials science, [2] as biologically active compounds [3] and very recently also in metallocsupramolecular chemistry [4]. In the field of synthesis and investigation of trinuclear cylindrical hexacarbon complexes, various works have been done experimentally. To the best of our knowledge, theoretical studies on the bonding nature of trinuclear-like cylindrical hexacarbon complexes have been performed less. In this structure project, the nature of the metal-ligand bonding of a number of cylindrical hexacarbon complexes such as trinuclears will be studied and the possibility of communicating between the theoretical and experimental data of these complexes will be investigated. By changing the central atom and replacing different d-block metals such as Cu(I), Ag(I), Au(I), Pd(II) and Hg(II) in the center of cylindrical hexacarbon complexes like trinuclears of these structural compounds, the stability and the nature of the bond in these compounds change significantly. To obtain the thermodynamic data of these compounds in the gas phase, calculations are performed on the optimized structures using the FREQ keyword. To investigate the nature of links and interactions, NBO, AIM and EDA calculations have been performed on the optimized structures with the PBEPBE methods and DEF2-TZVP basis set.

Keywords: NHC, Trinuclear, Cylindrical, Theoretical, FREQ

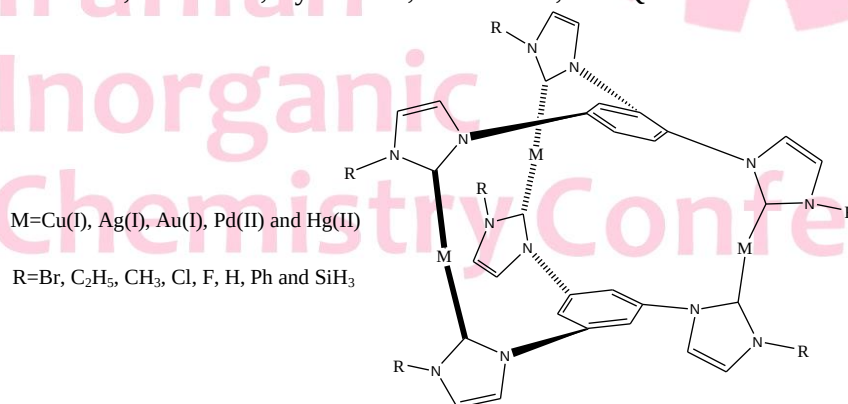


Figure 1: structure of trinuclear cylindrical hexacarbon complex

References

- [1] D. Enders, O. Niemeier, A. Henseler, *Chem. Rev.* **2007**, 107, 5606.
- [2] W. A. Herrmann, *Angew. Chem.*, **2002**, 41, 1290.
- [3] A. J. Boydston, K. A. Williams, C. W. Bielawski, *J. Am. Chem. Soc.* **2005**, 127, 12496.
- [4] K. M. Hindi, M. J. Panzner, C. A. Tessier, C. L. Cannon, W. J. Youngs, *Chem. Rev.* **2009**, 109, 3859.