

Abstract :

The thesis subject deals from a theoretical point of view with the mode of coordination and the electronic structure of transition metal complexes with carbenic ligands according to the nature of the metal. Several coordination sites are possible giving rise to several isomers classified between them according to their relative energies.

The calculation method used is the density functional theory (DFT) for the whole series of complexes studied; using the two programs; ADF using the TZP base and GAUSSIEN 09 using the base 6-31 ++ G ** with the hybrid functional groups B3LYP, B3PW91 and non-hybrid BP86, PW91PW91. Visualizations and representations of molecular structures were made using the Molden, Gaussview and Molekel programs.

The manuscript covers four parts. The first is an introduction to density functional theory (DFT). The 2nd and 3rd part study the molecular and electronic structure of carbene and metal complexes of the type : $[M(CO)_2Cl(NHC)]$ of which M: (M = V, Mn, Co, Re and Rh) and NHC: (NHC= C_3N_2 , or $N_2H_6C_{11}O_2$) and the 4th part only talks about molecular structures of some copper complexes (Correlation study)

We have studied in all cases the different carbene-metal bonds, they have shown at the end that they are stronger in the elements moderately rich in electrons like: (Re) than in the elements rich in electrons like : (Cu) .

Keywords:

Functional Density - Electronic Structures- hybrid functional- non-hybrid functional