Topological Analysis of the Bonding in \([Ru_5(M_2-C_2)L(CO)_{13}]\) and \([Ru_4(M_2-C_2)L(CO)_{10}]\) Complexes (L=-(M-Sme)(M-Pph)_2) \\
Abdelghani May and Nadia Ouddai

Laboratoire Chimie des matériaux et des vivants: Activité, Réactivité  
Université El-Hadj Lakhdar Batna- Algérie  
Ouddai_nadia@yahoo.fr

The nature of the metal-metal and metal-carbon bonding interactions within the tetra- and penta-Ruthenium acetylide complex, \([Ru_4(M_2-C_2)L(CO)_{10}]\), (1) and \([Ru_5(M_2-C_2)L(CO)_{13}]\), (2), respectively, have been investigated using the present topological theories of the chemical bond, AIM and ELF. The electron density analysis within the framework of Atoms in Molecules (AIM) indicates that, in the first complex, there is only one bond path exists between the metal atoms Ru4 and Ru5, whereas, there is no direct bonding between the Ruthenium atoms in the second complex. On the other hand, The ELF analysis reveals that all Ru-C bonds, in both complexes, belong to closed-shell type interactions, and lead to a conclusion that the Ru-Ru bond is predominantly covalent. Moreover, the presence of the trisynaptic basins, in the first complex, points out a three-center bond connecting the Ruthenium atoms. Metal acetylide complexes are of both theoretical and practical interest, in particular, as their potential to form molecular wires [1-3], liquid crystals [4], electrical conductors [5] and other nano electronic devices [6]. In this context, Chris J. Adams et al [8], reported the synthesis and structural determination of a penta- and tetra-Ruthenium acetylide complex, \([Ru_5(M_2-C_2)L(CO)_{13}]\), (1) and \([Ru_4(M_2-C_2)L(CO)_{10}]\), (2), respectively. Where L denotes the (μ-SMe)(μ-PPh)_2 group.

REFERENCES