Chapter 5
Closed Metal Cycles in Clusters With Ligands

ABSTRACT

This chapter considers closed three-membered metal cycles of one or several chemical elements surrounded by ligands connected to them. It has been proven that the widespread opinion in the literature about the formation of ligands by atoms in some cases of the semi-correct polyhedron of the anti-cube-octahedron is wrong. Geometrical analysis of the interpenetration of the coordinates of ligand atoms around each of the metal atoms of a closed chain showed that this leads to a different class of special three-dimensional irregular polyhedrons for different clusters. In all cases of homo-element and hetero-element closed metal chains, the cycle itself, located in a certain plane, creates a cross section of the cluster, dividing the cluster into two parts. Each of the parts of a cluster has dimension 4.

INTRODUCTION

Cluster compounds containing a skeleton in the form of metal cycles are a widespread type of cluster metal compounds (Gubin, 2019). Homo - cyclic structures with metal atoms from 3 to 8, bicyclic formations are known. Particularly, systems consisting of several condensed metal cycles can be considered. Cluster compounds that have one hundred in the form of three -membered metal cycles are obtained for most metals and have ligands of various types. In cluster compounds with a large number of metal atoms, the

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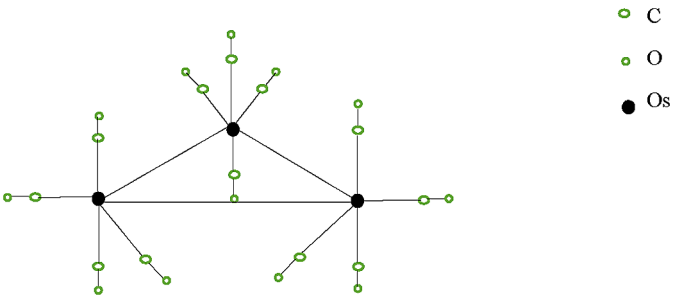
main part of the faces of the metal frame polyhedrons is triangles. Therefore, three - membered metal rings to some extent can simulate the properties of more complex clusters.

HOMO: ELEMENT METAL CYCLES WITH LIGANDS

The absence of bridging ligands and high symmetry make three - nuclear carbonyls $Ru_3(CO)_{12}$, $Os_3(CO)_{12}$ convenient support compounds for structural and theoretical studies of three - membered homo - element metal cycles. In molecules, each metal atom is associated with four functional groups (Figure 1).

Figure 1. Shema of three - nuclear carbonyls Ru and Os



It is believed that 12 ligands are arranged so that they form an anti – cube – octahedron as a ligand polyhedron (Mason & Rae, 1968; Benfield & Jonson, 1981; Gubin, 2019). However, evidence of this assumption has not yet been provided. The proof of this assertion could be a concrete construction of an anti – cube – octahedron with a three - link metal cycle enclosed in it, connection by valence bonds of the metal cycle atoms to the vertices of the anti – cube - octahedron. After this, it is required to determine the partition of the anti – cube - octahedron with the constructed valence bonds into elementary three - dimensional cells and the verification of the implementation of the Euler – Poincaré (Poincoré, 1895) equation for the constructed polytope. No such evidence was carried out. In this chapter, this question will be considered as part of the proof of the following theorem: