Chapter 4
Chains of Metallic Clusters With Ligands

ABSTRACT

This chapter geometrically investigated the structure of clusters, the core of which represent the metal chains (linear or curved) of both identical and different elements. It was shown that the dimension of the structures of these clusters is more than three. To create a model of these chains in a higher dimension space, a new geometric approach has been developed that allows us to construct convex, closed polytopes of these chains. It consists of removing part of the octahedron edges necessary for constructing the octahedron and adding the same number of new edges necessary to build a closed polytope chain while maintaining the number of metal atoms and ligands and their valence bonds. As a result, it was found that metal chain polytopes consist of polytopes of higher dimension, adjacent to each other along flat sections.

INTRODUCTION

Models containing polymetallic chains formed by metal atoms with ligands attached to them represent a special class of multicore clusters. Experimentally (Gubin, 2019) obtained a significant number of such compounds in the form of metal chains (usually three - link chains). Metal chains can be both homo - element and hetero - element, and the structure of the metal chain can be linear and non - linear (curved). Binuclear compounds with a metal - metal bond is partially consecrated in the monograph Cotton, Walton (1982). From short

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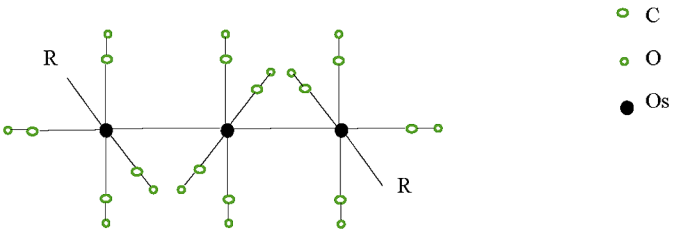
chains, as from bricks, longer metal chains can be constructed. In addition, the formation of polymeric compounds is possible, the main chain in which is built of metal atoms linked together.

In this monograph, it is of interest to determine the dimensionality of the chains of metal clusters with ligands. The methods for analyzing the geometry of high - dimensional polytopes, developed by the author (Zhizhin, 2018, 2019a, b), are used.

LINEAR HOMO - ELEMENT METAL CHAINS

An example of a linear homo - element metal chain is shown in Figure 1 (Smart, Cook, & Woodward, 1977; Evans, Okrasinski, Pribula, & Norton, 1976; Gochin & Moss, 1980).

Figure 1. Schematic structure of cluster connection $Os_3(CO)_{12}R_2$



In this example, we illustrate the sequence of actions to calculate the dimension of the metal chain. When determining the dimension of metal chains, atoms that are linearly located and do not have branching of the chain at their location do not matter (Zhizhin, 2018). At the same time, not only metal atoms, but also ligand atoms are of importance for determining the dimension of a compound. Therefore, Figure 1 can be represented as Figure 2.

In Figure 2, the red edges correspond to chemical bonds, and the black edges serve only to create a convex closed figure. It can be seen that each link of the metal chain creates an octahedron with the center as a convex figure. Moreover, the center of each octahedron is simultaneously the vertex of another neighboring octahedron or two neighboring octahedrons. In Figure