Chapter 6
Metallic Clusters With Ligands and Polyhedral Core

ABSTRACT

The geometry of clusters with ligands and a polyhedral frame is considered by the methods of studying the geometry of higher-dimensional polytopes, developed in the author's monograph. It is shown that these methods allow us to establish important details of cluster geometry, which elude analysis based on the representations of three-dimensional geometry. It is established that the well-known Kuban cluster is a 4-cross-polytope, which allows different variants of the Kuban cluster. A cluster of gold with a tetrahedral backbone is a 5-cross-polytope. The cluster tetra anion of cobalt is a polytope of dimension 5 of a new type. Different types of ligands limit the cobalt skeleton from above and below.

INTRODUCTION

A significant part of the known cluster are molecules that have a skeleton in the form of a metal polyhedron. In other words, the shortest distances between metal atoms in such molecules form a convex closed polyhedron bounded by flat faces. As a rule, these polyhedrons are considered three - dimensional. Even if in the simplest cases this is so, then taking into account the ligands attached to the skeleton, such a molecule will have a dimension greater three. In addition, the metal core may have a higher dimension, which further increases the dimension of the cluster. Therefore to analyze

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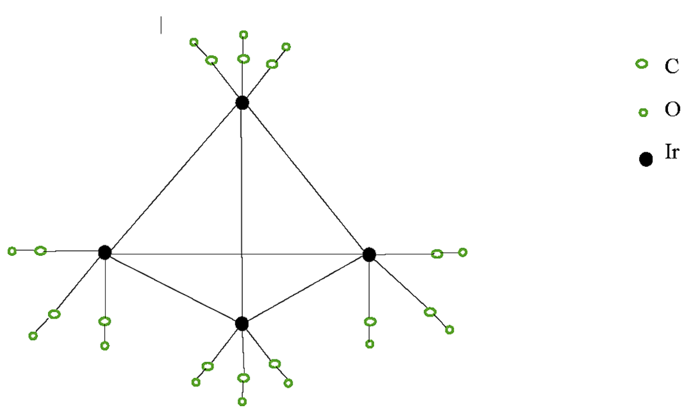
the structure of clusters with a metal backbone in the form of a polyhedron, it is necessary to use the geometry of high - dimensional polytopes, not the abstract geometry of spaces of higher dimension, but the geometry of high - dimensional polytopes based on the analysis of the geometry of chemical compounds (Zhizhin, 2018, 2019a, b). If the space surrounding the cluster is considered three - dimensional, the outer surface of the cluster can be constructed from two - dimensional faces, although the cluster itself has a higher dimension. The existence of a higher dimension space inside a three - dimensional space does not contradict the Riemann geometry (Riemann, 1854), since according to the Riemann geometry, space is finite (in Euclidean geometry the space is infinite).

Inside the cluster can meet a variety of convex bodies with dimensions less than the dimension of the cluster, including regular, semi - correct and irregular three - dimensional polyhedrons. Analysis of the structure of clusters, taking into account its dimensions and the dimensions of its components, is necessary for an adequate modern description of cluster geometry.

CLUSTER COMPOUNDS HAVING A SKELETON IN THE FORM OF A METAL TETREHEDRON

Among a wide variety of clusters, a special place is occupied by compounds based on the skeleton in the form of the simplest metal - polyhedron — the tetrahedron. Tetrahedral cluster compounds are widely distributed (Cubin, 2019; Garner, 1980). The special significance of tetrahedral clusters lies in

Figure 1. Homo - metallic tetrahedral iridium cluster $Ir_4(CO)_{12}$



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