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The Geometry of Higher-Dimensional Multi-Shell Clusters With Common Center and Different Centers:

The Geometry of Metal Clusters With Ligands

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ABSTRACT

In this article, it is shown that the dimension of a metal skeleton of giant palladium cluster, containing 561 atoms in five shells, is 8. The claims of some authors that the palladium cluster in this case is an E8 lattice are groundless. The internal geometry of multi-shell metal clusters with ligands and core was investigated. It is proved that the multi-shell clusters with common center and different centers have a higher dimension. Clusters with ligands and a structural unit octahedron exist with different metals in the core. A spatial image of the cobalt tetra-anion cluster is presented. It is proved that its dimension is 5. It is considered homo-element metal cycles with ligands. For example, a spatial image of the three nuclear carbonyls of ruthenium and osmium it is build. It was proved that the ligands in the three nuclear carbonyls of ruthenium and osmium do not form a ligand polyhedron, as was previously assumed. The construction of cluster in this case can be divided into two polytopes dimension of 4.

KEYWORDS

Cluster, Cuboctahedron, Dimension, Edge, Face, Icosahedron, Octahedron, Polytope, Tetrahedron, Vertices

INTRODUCTION

In a recent work of the author (Zhizhin, 2019a) higher dimensions of clusters of intermetallic compounds were considered. In particular, multi-shell intermetallic clusters were considered, each shell of which is a convex regular three-dimensional polyhedron (Plato bodies). It was assumed that all shells in a certain arbitrary cluster have a common center and are of the same type. The statement is proved.

Theorem: The dimension d of a cluster of N shells with a common center is $N + 2$, if there is no atom in the common center, and is equal to $N + 3$, if there is an atom in the common center.

The proved statement allows us to calculate the dimension of many well-known intermetallic clusters: Mackay, Bergman, Samson, and others (Mackay, 1962; Pauling, 1960; Nyman & Anderson,1979; Bergman et al., 1952, 1957; Komura et al., 1960; Audier et al., 1998; Samson, 1972).

Continuing the mathematical descriptions begun in this work of real clusters of chemical compounds with the determination of their dimension, this article discusses multi-shell metal clusters

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with ligands. Moreover, the shells in one cluster may have a different shape, as well as a common center or several centers at the same time. The study is based on the classification of various real clusters of chemical compounds with ligands (Gubin, 2019). This line of research is fundamentally different from abstract cluster studies that are not associated with specific chemical compounds and do not have technological significance (McMullen, & Schulte, 2002; Diudea & Nagy, 2007; Ashrafi, Cataldo, Iraumanesh, & Ori, 2013; Diudea, 2018).

THE DIMENSION OF A METAL SKELETON OF GIANT PALLADIUM CLUSTER

It was shown (Vargaftik, et al., 1985) that upon the reduction of palladium acetate with hydrogen in the presence of nitrogen-containing ligands (L), polynuclear complexes are formed, which are easily converted into cluster compounds. Based on the study of their structure by electron microscopy, they were assigned the composition $Pd_{561}L_{60}(O_2)_{180}(OAc)_{180}$. The palladium atoms in this compound form a dense packing in the form of five icosahedrons with a common center in which the palladium atom is located. Ligands are located on the surface of a metal skeleton. The number of atoms in the metal core of this cluster is determined by the formula:

$$1+\sum_{1}^{N}(10N^2+2), N$$

is the number of layers around the central metal atom (Lord et al., 2006).

From Theorem in introduction (Zhizhin, 2019 a) at once it follows that the dimension of a metal skeleton of giant palladium cluster, containing 561 atoms in five shells, is 8. The claims of some authors that the palladium cluster in this case is an E_8 lattice (Shevchenko, 2011) are groundless. The lattice E_8, as you know (Conway, & Sloane, 1988), is a collection of points in an eight-dimensional space with coordinates $(\pm 1, \pm 1, 0, 0, 0, 0, 0, 0)$, where units can stand anywhere on the line with arbitrary signs, as well as points with coordinates:

$$(\pm\frac{1}{2},\pm\frac{1}{2},\pm\frac{1}{2},\pm\frac{1}{2},\pm\frac{1}{2},\pm\frac{1}{2},\pm\frac{1}{2},\pm\frac{1}{2})$$

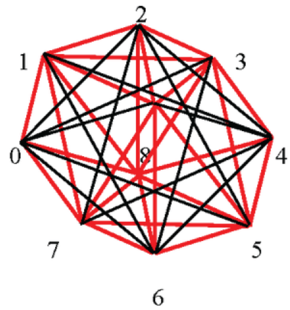
Obviously, this lattice has nothing to do with the structure of a cluster consisting of five icosahedral shells. It is assumed (Coxeter, 1963) that the lattice E_8 corresponds to the polytope of Gosset (Gosset, 1900), which draws from simplexes and cross-polytopes. But from the previous it follows that the polytope corresponding to the metal skeleton of a giant palladium cluster does not include either simplexes or cross-polytopes.

CLUSTERS ON AN OCTAHEDRON

Let there be a set of six atoms of osmium bound by a chemical bond (Gubin, 2019). The addition of other osmium atoms to this structure occurs by centralizing the planar triangular faces of the octahedron. As the first stage, atoms attach to triangular faces (located above them on the outside of the octahedron). In this case, faces with attached atoms and faces with non-attached atoms alternate with each other. Since four atoms joined the octahedron, a cluster of ten atoms forms (Figure 1).

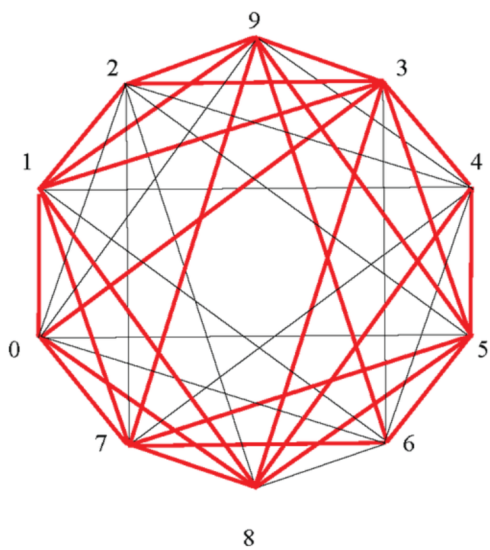
In order to represent this cluster in the form of a convex figure, it is necessary to supplement it with edges. In this case, for the formation of a convex closed figure, the minimum additional

Figure 1. The octahedron with attached tetrahedrons on faces of octahedron



number of edges is 16 (black segments in Figure 1). In a topologically equivalent form, this cluster is depicted in Figure 2.

Figure 2. The 5 – cross - polytope



You can see that this is a 5 - cross - polytope. Each vertex in Figure 2 is connected by an edge to all other vertices with the exception of the opposite vertex. The number of elements of the dimension *i* in the *d* - cross - polytope is equal (Zhizhin, 2013, 2014, 2018, 2019 b):

$$f_i = 2^{1+i} C_d^{d-1-i} \tag{1}$$

It have 10 vertices $\left(f_0(5) = 2^{1+i} C_4^5 = 10\right)$, 40 edges $\left(f_1(5) = 2^2 C_5^3 = 40\right)$, 80 triangle faces $\left(f_2(5) = 2^3 C_5^2 = 80\right)$, 80 tetrahedrons $\left(f_3(5) = 2^4 C_5^1 = 80\right)$, 32 four – dimensional simplexes

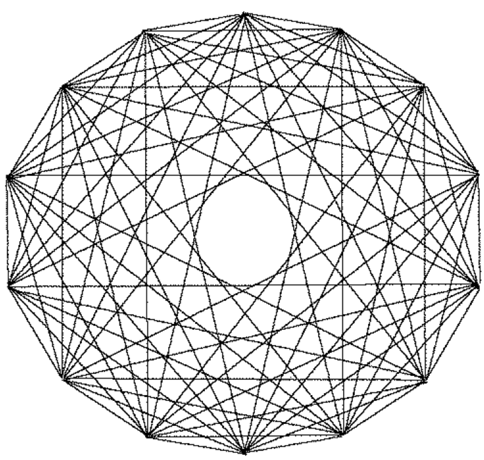
$\left(f_4(5) = 2^5 = 32\right)$. The dimension of a figure is determined by the Euler-Poincare equation (Poincare, 1895):

$$\sum_{i=0}^{d-1} (-1)^i f_i(P) = 1 + (-1)^{d-1} \tag{2}$$

In (2) $f_i(P)$ is the number of faces with dimension *i* in polytope *P* with dimension *d*.

Including the numbers f_i in equation (2) we get 10 – 40 + 80 – 80 + 32 = 2. This proves that the figure in Figure 2 is a convex polytope of dimension 5. It is easy to make sure that with fewer edges the complex of ten atoms will not be convex, since equation (2) will not be satisfied. The next step in the formation of a cluster as a convex figure could be the attachment of atoms to the faces of the octahedron to which the atoms have not yet been attached. There are four such free faces. However, as follows from Figures 1 and 2, when constructing a convex figure, these free faces turned out to be already occupied tetrahedra without changing the number of vertices. But the edges of these tetrahedra have only geometric meaning for creating a convex figure. Therefore, attachment to these faces of tetrahedra with chemical bonds is still possible. Then a figure with 14 vertices is formed. Creating a convex figure from it will lead to the formation of a 7 - cross - polytope, which has already been shown in Figure 3.

Figure 3. The 7 – cross - polytope



From the general expression for the number of elements of the dimension and in the *d* - cross - polytope (1) it follows that the number of vertices in this polytope $f_0 = 2 \cdot C_7^6 = 14,$ the number of edges $f_1 = 2^2 \cdot C_7^5 = 84,$ the number of triangle faces $f_2 = 8 \cdot C_7^4 = 280,$ the number of tetrahedrons $f_3 = 16 \cdot C_7^3 = 560,$ the number of four - dimension simplexes $f_4 = 32 \cdot C_7^2 = 672,$ the number of five - dimension simplexes $f_5 = 64 \cdot C_7^1 = 448,$ the number of six - dimension simplexes $f_6 = 128.$ Further attachment of atoms to the 7 - cross - polytope can be limited by the possibility of creating a large number of valence bonds.

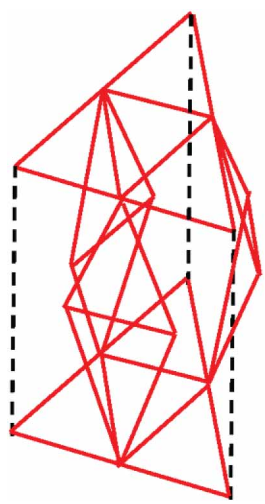
CLUSTERS ON A CUBOCTAHEDRON

Let there be a set of 12 rhodium atoms linked by a chemical bond, forming one of the forms of the cuboctahedron (Figure 4).

Figure 4. The Cuboctahedron

6 other rhodium atoms can join this design by centering the square faces. Geometrically, this means joining to the square faces of the cuboctahedron 6 quadrangular pyramids on the outside of the cuboctahedron. In this case, a figure is formed having two parallel triangular faces, each of which is composed of four triangular sections. In the center of the parallel faces of the figure is the triangular faces of the cuboctahedron. In order to create a convex figure, in this case it is enough to connect the corresponding vertices of these parallel faces with the edges (Figure 5).

Figure 5. The "bloated" prism

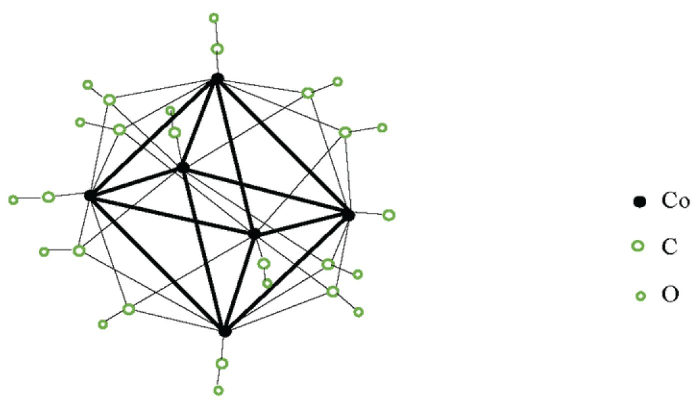


The sides of the resulting figure contain two trapezoids tilted to each other. Each of them is composed of three triangles. So that the sides of the figure are not flat. We can say that the resulting figure is a "bloated" prism. Each of the three generators of this prism is simultaneously the edges of three tetrahedrons that close the figure. So, the resulting figure contains 12 vertices of the cuboctahedron and 6 vertices of the attached six pyramids, i.e. $f_0 = 18$. Many edges of the figure contain 24 edges of the cuboctahedron, 24 edges of the attached pyramids and 3 edges of the generators, i.e. $f_1 = 51$. The flat sections of this figure are composed of 14 flat faces of the cuboctahedron, 24 triangular faces of the pyramids and 6 flat faces of the tetrahedra containing 3 generators, i.e. $f_2 = 44$. The figure includes 11 three-dimensional bodies (6 pyramids, 3 tetrahedrons, 1 cuboctahedron, 1 three-dimensional body with the outer surface of the figure without taking into account the internal content of the figure, i.e. $f_3 = 11$. Substituting these numbers into the equation (2) we get 18 – 51 + 44 – 11 = 0. This proves that the resulting figure has dimension four. It should be noted that the figure obtained is an example of a polytope of higher dimension significantly different from a simplex and a cross-polytope. As follows from the construction (Figure 5), 5 edges come from each of its six vertices, which are simultaneously the vertices of the attached pyramids. From any of the other vertices that coincide with the vertices of the cuboctahedron, 6 edges emanate. While in a simplex with 18 vertices, 17 edges emanate from each vertex, and in a cross-polytope, under the same conditions, 16 edges emanate from each vertex. Further addition of atoms will increase the dimension of the figure, provided it is convex.

COMPOUNDS WITH LIGANDS HAVING A METAL OCTAHEDRON FRAME

Clusters with ligands and a structural unit octahedron exist with different metals in the core: Pt, Pd, Ni, Cu, Ti, Fe, Ru and other metals (Gubin, 2019). They are distinguished by sufficient structural complexity, leading to the formation of polytopes of a higher dimension of new types. So far, none of them have been analyzed in the space of higher dimension. As an illustration of such an analysis, we consider the structure of the cobalt tetra - anion cluster $[Co_6(\mu - Co)_8(CO)_6]^{4-}$. The scheme of this compound is shown in Figure 6 (Johnson, & Benfield, 1981).

Figure 6. Scheme of cobalt tetra - anion cluster $[Co_6(\mu - Co)_8(CO)_6]^{4-}$

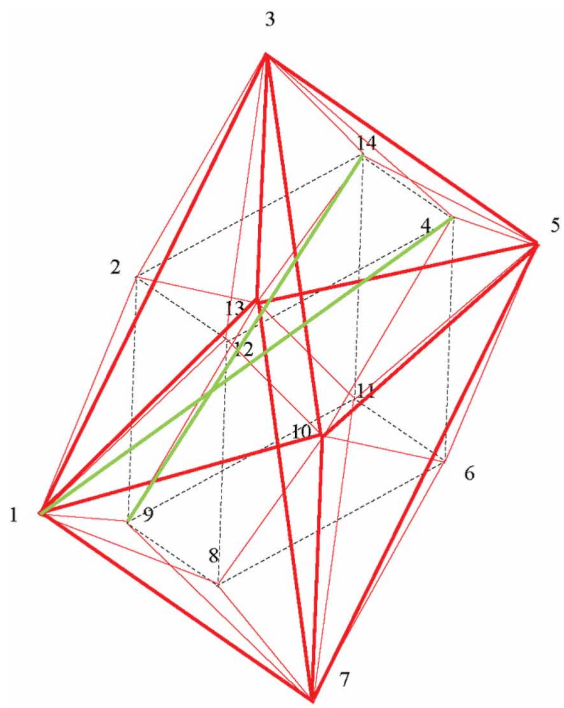


The desire to create a convex model of this compound leads to the appearance of various three -dimensional polyhedrons and four - dimensional polytopes entering into each other.

Theorem 1: The dimension of cobalt tetra - anion cluster $[Co_6(\mu - Co)_8(CO)_6]^{4-}$ equal 5.

Proof: To build a spatial model of cobalt tetra - anion cluster $[Co_6(\mu - Co)_8(CO)_6]^{4-}$, let us turn to its scheme in Figure 6. From this figure, it can be seen that the ligands (μ - CO) that bind two metal atoms form a cube. In addition, each vertex of the metal core in the form of an octahedron is formed as a result of constructing a pyramid on each face of the ligand cube. The free vertices of these pyramids give the vertices of the octahedron of atoms cobalt. The six faces of the cube thus give six vertices of the octahedron. Consider first the figure that forms as a result of this construction. The spatial image of this figure is shown in Figure 7.

Figure 7. The spatial image of compound $Co_6(\mu - Co)_8$



The valence bonds are indicated in this figure with red edges. The edges of the ligand cube are marked with dotted black lines. The edges of the pyramids, with the exception of the grounds, denoted by solid lines in black. Thus, the ligands (μ - CO) are located at the vertices 2, 4, 6, 8, 9, 11, 12, 14. Metal atoms are located at the vertices 1, 3, 5, 7, 10, 13. To create a closed convex figure in the figure, two edges are added blue 1 - 4, 9 - 14. Determine the dimension of this compound. There are 14 vertices here $(f_0 = 14)$. The numbers of edges on Figure 7 is 50 ($f_1 = 50)$:

1 - 2, 1 - 3, 1 - 13, 1 - 12, 1 - 4, 1 - 10, 1 - 9, 1 - 8, 1 - 7, 2 - 3, 2 - 13, 2 - 14, 2 - 12, 2 - 9, 3 – 4, 3 - 5, 3 - 14, 3 - 13, 3 - 12, 3 - 10, 4 - 5, 4 - 6, 4 - 10, 4 - 12, 4 - 14, 5 - 14, 5 - 11, 5 - 10, 5 - 6, 5 - 7, 5 - 13, 6 - 7, 6 - 10, 6 - 11, 6 - 8, 7 - 10, 7 - 11, 7 - 13, 7 - 8, 7 - 9, 8 - 9, 8 - 10, 8 - 12, 9 - 11, 9 - 13, 9 - 14, 10 - 12, 11 - 13, 11 - 14, 13 – 14

The number of triangles on Figure 7 is 58:

1 - 2 - 3, 1 - 3 - 13, 1 - 3 - 12, 1 - 2 - 13, 1 - 2 - 12, 1 - 2 - 9, 1 - 9 - 8, 1 - 9 - 7, 1 - 12 - 8, 1 - 13 - 7, 1 - 10 - 7, 1 - 10 - 8, 1 - 10 - 12, 1 - 10 - 3, 1 - 9 - 13, 1 - 8 - 7, 2 - 12 - 3, 2 - 13 - 3, 2 - 14 - 3, 2 - 14 - 13, 2 - 9 - 13, 3 - 12 - 4, 3 - 13 - 14, 3 - 13 - 5, 3 - 4 - 5, 3 - 14 - 5, 3 - 14 - 4, 3 - 10 - 12, 3 - 10 - 4, 3 - 10 - 5, 4 - 5 - 14, 4 - 10 - 12, 4 - 5 - 10, 4 - 6 - 10, 4 - 5 - 6, 5 - 13 - 11, 5 - 13 - 14, 5 - 14 - 11, 5 - 11 - 6, 5 - 11 - 7, 5 - 10 - 6, 5 - 7 - 6, 5 - 10 - 7, 6 - 10 - 7, 6 - 11 - 7, 6 - 8 - 7, 6 - 8 - 10, 7 - 11 - 13, 7 - 8 - 10, 7 - 8 - 9, 7 - 9 - 11, 7 - 9 - 13, 8 - 10 - 12, 9 - 11 - 13, 9 - 13 - 14, 9 - 14 - 11, 1 - 12 - 4, 1 - 10 – 4

The number of tetragon flat faces on Figure 7 is 6:

2 - 14 - 4 - 13, 14 - 4 - 11 - 6, 11 - 6 - 8 - 9, 9 - 8 - 2 - 13, 4 - 6 - 8 - 12, 2 - 14 - 11 - 9

Thus, the common number of flat faces on Figure 7 is 64 $(f_2 = 64)$. The number of tetrahedrons on Figure 7 is 19:

1 - 2 - 3 - 12, 1 - 12 - 9 - 7, 1 - 12 - 8 - 9, 1 - 2 - 3 - 13, 1 - 2 - 12 - 9, 1 - 3 - 11 - 13, 1 - 9 - 8 - 7, 2 - 12 - 14 - 3, 3 - 4 - 5 - 14, 3 - 13 - 4 - 11, 13 - 8 - 11 - 1, 4 - 5 - 6 - 11, 5 - 14 - 10 - 12, 5 - 11 - 7 - 6, 5 - 10 - 7 - 6, 5 - 12 - 7 - 10, 6 - 11 - 7 - 8, 7 - 9 - 10 - 12, 1 - 8 - 11 – 7

The number of pyramids on Figure 7 is 6:

2 - 12 - 4 - 6 - 3, 4 - 14 - 6 - 11 - 5, 6 - 8 - 9 - 11 - 7, 9 - 8 - 12 - 2 - 1, 4 - 6 - 8 - 12 - 10, 2 - 14 - 11 - 9 - 13

On Figure 7 is 1 cube:

2 - 14 - 4 - 12 - 6 - 8 - 9 – 11

and is 1 octahedron:

1 - 3 - 5 - 7 - 10 – 13

In addition, in Figure 7 there is also a closed body with 12 vertices:

2 - 13 - 11 - 10 - 6 - 12 - 3 - 5 - 1 – 7

His image is presented separately in Figure 8.

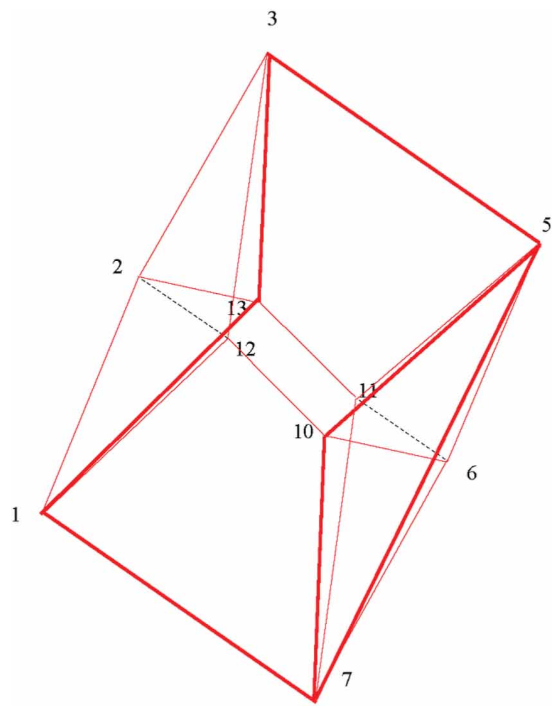
Determine the dimension of the body S. For this body is $f_0 = 10$. The number of edges on Figure 8 is 22 $(f_1 = 22)$:

1 - 2, 1 - 13, 1 - 12, 1 - 10, 1 - 7, 2 - 3, 2 - 13, 2 - 12, 3 - 5, 3 - 10, 3 - 13, 3 - 12, 5 - 13, 5 - 11, 5 - 10, 6 - 7, 6 - 10, 6 - 11, 7 - 10, 7 - 11, 10 - 12, 11 – 13

The number of triangles on Figure 8 is 8:

2 - 3 - 12, 2 - 3 - 13, 1 - 2 - 13, 6 - 5 - 10, 6 - 5 - 11, 1 - 2 - 12, 7 - 6 - 10, 7 - 6 – 11

Figure 8. The image a closed body S = 2 - 13 - 11 - 10 - 6 - 12 - 3 - 5 - 1 - 7



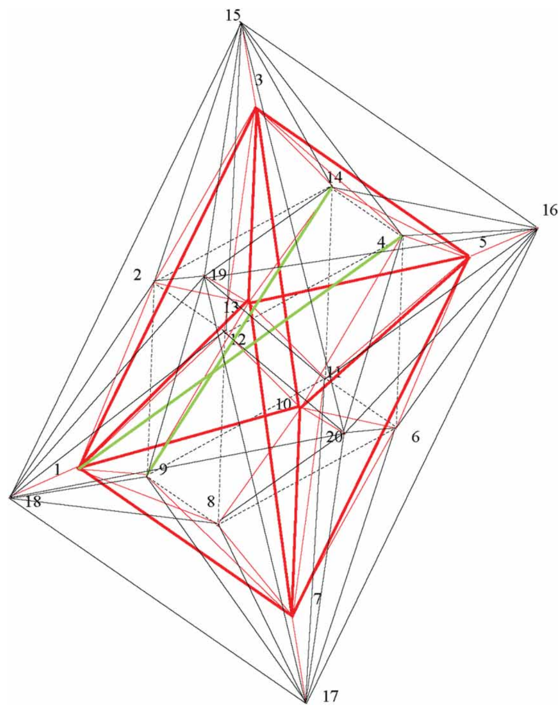
The number of tetragon flat faces on Figure 8 is 4:

13 - 3 - 5 - 11, 12 - 3 - 5 - 10, 1 - 7 - 13 - 11, 1 - 12 - 10 – 7

Thus, the common number of flat faces on Figure 8 is 12 $(f_2 = 12)$. Substituting the obtained values $f_i(i = 0,1,2)$ in the equation (2) you can see that the Euler - Poincaré equation is satisfied in his case for n = 3 10 – 22 + 12 = 2. This proves that Figure 8 is polyhedron with dimension 3. Consequently, the total number of three - dimensional figures included in the polytope in Figure 7 is $19 + 9 = 28$, i.e. for this figure $f_3 = 28$. Substituting the obtained for Figure 7 values $f_i(i = 0,1,2,3)$ in the equation (2) you can see that the Euler - Poincaré equation is satisfied in his case for n = 4 14 – 50 + 64 – 28 = 0. This proves that Figure 7 is polytope with dimension 4. Now back to the review of cobalt tetra - anion cluster $[Co_6(\mu - Co)_8(CO)_6]^{4-}$ in Figure 6. On Figure 7 shows the spatial image of only part of this compound. To create the spatial image of this compound, it is necessary to release the edges into the outer part from the vertices of the octahedron in Figure 7 and build a larger octahedron 15 - 16 - 17 - 18 - 19 - 20 on the free vertices of these edges. This are red edges 1 - 18, 3 - 15, 5 - 16, 7 - 17, 13 - 19, 10 - 20 on Figure 9.

Thus, the number of vertices on Figure 9 equal 20 $(f_0 = 20)$. The construction of a large octahedron taking into account the edges connecting two octahedrons adds 16 edges to the body in Figure 7. A three - dimensional figure is formed between each face of a large octahedron and the corresponding face of a small octahedron. For example, a three - dimensional figure is formed between the face of 1 - 10 - 7 small octahedron and the face 18 - 17 - 20 of the large octahedron (see Figure 9) 1 - 10 - 7 - 18 - 17 - 20. The number of such three - dimensional figures is equal to the number of faces of the octahedron - 8. In addition, to fill the space between the large octahedron and other

Figure 9. Spatial image of cobalt tetra - anion cluster $[Co_6(\mu - Co)_8(CO)_6]^{4-}$



convex bodies that make up the polytope in Figure 7, it is necessary to connect the vertices of the large octahedron with the vertices of the cube:

2 - 14 - 4 - 12 - 6 - 8 - 9 – 11

This adds to the body in Figure 7 another 24 edges:

2 - 15, 12 - 15, 14 - 15, 4 - 15, 14 - 16, 4 - 16, 6 - 16, 11 - 16, 6 - 17, 8 - 17, 9 - 17, 11 - 17, 8 - 18, 9 - 18, 2 - 18, 12 - 18, 2 - 19, 14 - 19, 9 - 19, 11 - 19, 4 - 20, 12 - 20, 8 - 20, 6 – 20

Thus, a common number of the edges on Figure 9 is $50 + 16 + 24 = 90$ $(f_1 = 90)$. The construction of a large octahedron taking into account the edges connecting two octahedrons adds 20 flat faces to body on Figure 7. Connection the vertices of the large octahedron with the vertices of the cube adds 48 flat faces to Figure 7. For example, the face of the cube:

2 - 14 - 4 – 12

when building a large pyramid on it gives an additional 8 flat faces:

2 - 12 - 15, 4 - 12 - 15, 4 - 14 - 15, 2 - 14 - 15, 12 - 3 - 15, 2 - 3 - 15, 4 - 3 - 15, 14 - 3 – 15

Since the faces at cube 6 one gets an additional 48 flat faces. In this way, the total number of flat edges in Figure 14 is 64 + 20 + 48 = 132, $(f_2 = 132)$. The construction of a large octahedron taking into account the edges connecting two octahedrons adds 9 three - dimensional faces to body on Figure 7. Connection the vertices of the large octahedron with the vertices of the cube adds 30 three - dimensional faces to Figure 7. For example, the face of the cube:

2 - 14 - 4 – 12

when building a large pyramid on it gives an additional 5 three - dimensional faces:

2 - 12 - 15 - 3, 4 - 12 - 15 - 3, 4 - 14 - 15 - 3, 2 - 14 - 15 - 3, 12 - 2 - 15 - 4 – 14

Since the faces at cube 6 one get an additional 30 three - dimensional faces. In addition, 4 tetrahedrons are additionally formed between the cube and the large octahedron, each of which has an edge of one of the edges of a rectangular cross section of:

15 - 16 - 17 – 18

large octahedron. For example, a tetrahedron:

18 - 17 - 8 – 9

is formed on the edge 17 - 18. Thus, the total number of three - dimensional areas in the body in figure 14 is 28 + 9 + 30 + 4 = 71 $(f_3 = 71)$. Connection the vertices of the large octahedron with the vertices of the cube adds 2 four - dimensional faces to Figure 7, one of which has an edge 18 - 17 and second has edges 15 - 16 of a rectangular cross section of:

15 - 16 - 17 – 18

large octahedron. For example, on the edge 17 - 18 formed area 18 - 1 - 9 - 8 - 7 - 17 (see Figure 9). This area has 6 vertices $(f_0 = 6)$. It has14 edges $(f_1 = 14)$:

1 - 9, 1 - 8, 1 - 7, 1 - 18, 7 - 8, 7 - 9, 7 - 17, 8 - 9, 8 - 18, 8 - 17, 9 - 18, 9 - 17, 9 - 8, 18 – 17

It has 14 two - dimensional faces $(f_2 = 14)$:

1 - 9 - 18, 1 - 9 - 8, 1 - 8 - 7, 1 - 7 - 17 - 18, 7 - 9 - 17, 7 - 8 - 9, 7 - 9 - 17, 8 - 17 - 18, 8 - 9 - 17, 8 - 9 - 18, 9 - 18 – 17

It has 6 three - dimensional faces $(f_3 = 6)$:

1 - 9 - 8 - 18, 1 - 9 - 8 - 7, 18 - 9 - 8 - 17, 1 - 18 - 9 - 7 - 17, 9 - 8 - 7 - 17, 1 - 8 - 18 - 7 – 17

Substituting the obtained for Figure 7 values $f_i (i = 0,1,2,3)$ in the equation (2) you can see that the Euler - Poincaré equation is satisfied in his case for $n = 4$ 14 – 50 + 64 – 28 = 0. This proves that body 18 - 1 - 9 - 8 - 7 - 17 is polytope with dimension 4. It is also proved that the body 15 - 16 - 5

- 4 - 14 - 3 has the dimension 4. It can be shown that, due to the orientation of the cube with respect to the large octahedron, similar four - dimensional polytopes with the edges of the large octahedron 18 - 15 and 17 - 16 do not form. Connection the vertices of the large octahedron with the vertices of the cube adds yet 6 four - dimensional faces to Figure 7, associated with the formation of structures of the pyramid in the pyramid on the faces of the cube. Consider for example two pyramids on the face of a cube:

2 - 12 - 14 – 4

This body has 6 vertices $(f_0 = 6)$, 13 edges $(f_1 = 13)$:

2 - 3, 2 - 15, 12 - 3, 12 - 15, 4 - 3, 14 - 3, 4 - 15, 14 - 15, 3 - 15, 2 - 12, 2 - 14, 4 - 12, 4 - 14, 13

two - dimensional faces $(f_2 = 13)$:

2 - 15 - 12, 2 - 3 - 12, 4 - 3 - 14, 4 - 15 - 14, 3 - 4 - 12, 15 - 4 - 12, 2 - 14 - 3, 2 - 14 - 15, 12 - 3 - 15, 2 - 3 - 15, 4 - 3 - 15, 14 - 3 - 15, 2 - 14 - 12 – 4

and 6 three - dimensional faces $(f_3 = 6)$:

2 - 14 - 4 - 12 - 3, 2 - 14 - 4 - 12 - 15, 4 - 3 - 15 - 14, 12 - 4 - 3 - 15, 2 - 12 - 3 - 15, 2 - 3 - 14 – 15

Substituting the obtained for two pyramids values $f_i (i = 0, 1, 2, 3)$ in the equation (2) you can see that the Euler - Poincaré equation is satisfied in his case for *n* = 4: 14 – 50 + 64 – 28 = 0. This proves that construction from two pyramids is polytope with dimension 4. The four - dimensional structure of two pyramids on the remaining five faces of the cube is proved in a similar way. In addition, the polytope in Figure 9 has two polytopes formed by inscribing a cube into an octahedron (large and small). Each of these polytopes has dimension 4 (this has already been proved). Finally, the polytope in Figure 9 has a polytope octahedron in an octahedron. This polytope also has dimension 4. Therefore, the total number of polytopes of dimension 4 that make up a polytope in Figure 9 is 11 $(f_4 = 11)$. Substituting the obtained for Figure 9 values $f_i (i = 0, 1, 2, 3, 4)$ in the equation (2) you can see that the Euler - Poincaré equation is satisfied in his case for *n* = 5 20 – 90 + 132 – 71 + 11 = 2. This proves that dimension of cobalt tetra - anion cluster $[Co_6 (\mu - Co)_8 (CO)_6]^{4-}$ equal 5. Q.E. D.

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 10).

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

(Poincaré, 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.

Theorem 2: The geometric model of three nuclear carbonyls Ru and Os consists of two polytopes of dimension 4, touching each other in a two - dimensional section, containing a three nuclear metal cycle.

Proof: Let us assume that carbonyl ligands form a ligand polyhedron in the form of an anti - cube - octahedron. Then the three nuclear metal cycle contained in an anti - cube - octahedron must be connected by vertices of an anti - cube - octahedron by valence bonds. Each vertex of the metal cycle must be connected with the four nearest vertices of the anti - cube - octahedron. In an arbitrary general form will look like that shown in Figure 11.

Figure 10. Shema of three - nuclear carbonyls Ru and Os

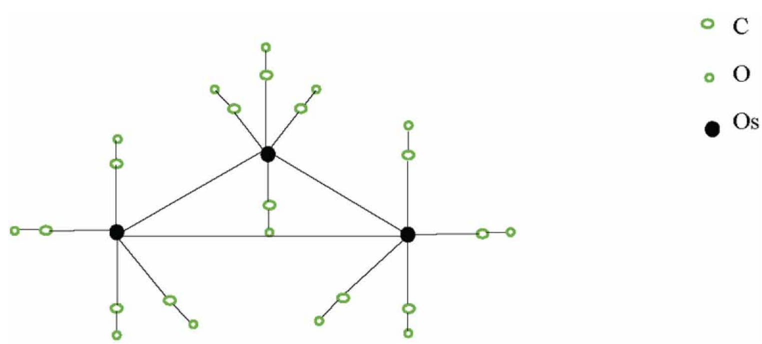
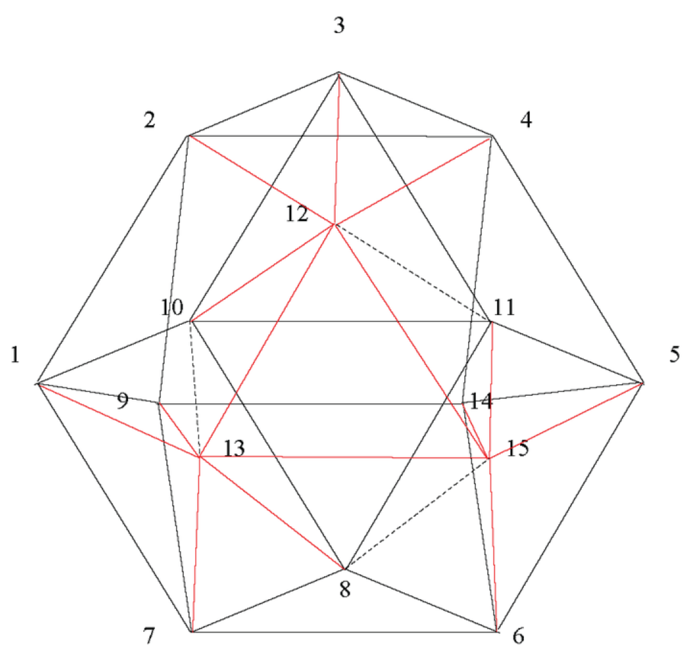


Figure 11. The anti - cube - octahedron with the three nuclear metal cycle



At the vertices 12, 13, 14, belonging to the metal cycle, there are metal atoms, and at the 12 vertices of the anti - cube - octahedron functional groups CO are present. The valence bonds of the metal atoms with each other and the functional groups are indicated by red edges. The edges of the anti - cube - octahedron is denoted by solid black lines. Valence bonds and edges of anti - cube - octahedron already create convex three - dimensional bodies:

2 - 3 - 4 - 12, 2) 5 - 6 - 15 - 14, 3) 1 - 9 - 13 - 7, 4) 9 - 12 - 13 - 14 - 15, 5) 1 - 2 - 12 - 9 - 13, 6) 3 - 4 - 12 - 11 - 5 - 15, 7) 4 - 12 - 5 - 15 - 14, 8) 2 - 4 - 9 - 14 - 12, 9) 7 - 9 - 14 - 6 - 13 - 15, 10) anti - cube - octahedron 1)

However, body particles do not yet create a partition of the space inside the anti - cube - octahedron into elementary three - dimensional cells, i.e. do not create the structure of this space. To create it, you need to add more edges between the 15 vertices of the system. You need to do this carefully enough so as not to come to possible contradictions. To do this, choose in the system the smallest possible number of places for holding these edges so that each added edge leads to the creation of the maximum number of three-dimensional bodies. Such places can be symmetrically located edges (indicated by dotted lines) 13 - 10, 12 - 11, 11 - 15. These edges lead to the creation of a whole series of three - dimensional bodies:

1-7 - 8 - 10 - 13, 12) 13 - 10 - 11 - 15 - 12 - 8, 13) 10 - 3 - 11 - 12, 14) 7 - 8 - 13 - 15 - 6, 15) 9 - 13 - 12 - 14 - 15, 16) 1 - 3 - 10 - 2 - 13 - 12, 17) 3 - 10 - 12 - 11, 18) 5 - 6 - 8 - 11 - 15 11)

Now the whole space of the anti - cube - octahedron is divided into three - dimensional polyhedrons.

Two numbers are already there $f_0 = 15, f_3 = 18$. It is necessary to count the number of edges and the number of flat two - dimensional elements. It is possible to determine that Figure 11 has 45 edges ($f_1 = 45)$:

1 - 2, 1 - 9, 1 - 10, 1 - 13, 1 - 7, 2 - 3, 2 - 4, 2 - 12, 2 - 9, 3 - 10, 3 - 12, 3 - 11, 3 - 4, 4 - 12, 4 - 14, 4 - 5, 5 - 11, 5 - 14, 5 - 15, 5 - 6, 6 - 14, 6 - 15, 6 - 8, 6 - 7, 7 - 8, 7 - 13, 7 - 9, 8 - 15, 8 - 10, 8 - 13, 8 - 11, 9 - 12, 9 - 14, 9 - 13, 10 - 12, 10 - 11, 10 - 13, 11 - 2, 11 - 15, 12 - 13, 12 - 14, 12 – 15, 13 - 15, 14 - 15

31 two - dimensional elements ($f_2 = 31)$ (two - dimensional elements that are a section of three -dimensional figures are not taken into account):

1 - 2 - 3 - 10, 1 - 2 - 9, 1 - 9 - 13, 1 - 10 - 13, 1 - 9 - 7, 2 - 3 - 4, 2 - 4 - 12, 2 - 4 - 9 - 14, 3 - 10 - 12, 3 - 10 - 11, 3 - 4 - 12, 3 - 4 - 5 - 11, 3 - 12 - 11, 4 - 14 - 12, 4 - 5 - 14, 5 - 14 - 15, 5 - 15 - 6, 5 - 14 - 6, 6 - 14 - 15, 5 - 6 - 8 - 11, 6 - 8 - 15, 7 - 8 - 6, 7 - 8 - 13, 7 - 9 - 13, 8 - 13 - 10, 8 - 11 - 15, 8 - 10 - 11, 1 - 7 - 8 - 10, 1 - 2 - 12 - 13, 9 - 12 - 13, 11 - 15 - 12

Substituting the obtained values $f_i (i = 0,1,2,3)$ in the equation (2) you can see that the Euler - Poincaré equation is not satisfied in this case:

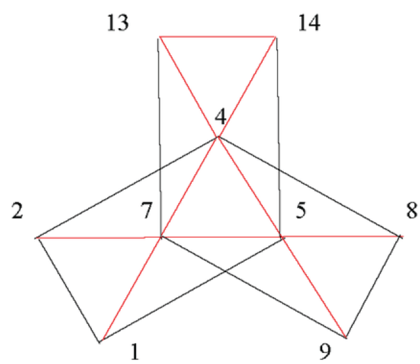
15 – 45 + 31 – 18 = - 17 < 0

This proves that Figure 11 is not polytope.

The reason for this lies in the fact that not all the flat faces of the 45 faces are the faces of two adjacent polyhedrons. It can be determined from Figure 11 that the faces 3 - 10 - 12, 3 - 12 - 11 are not at the same time the face of two neighboring polyhedrons (they are only a part of the face of neighboring polyhedrons). This is a necessary condition for the existence of a polytope in this case, dimension 4. With increasing polytope dimension, each flat face must simultaneously be the face of an even larger number of three - dimensional faces (Zhizhin, 2019 b). Attempts to draw additional edges in Figure 11, in order to create additional three - dimensional bodies with faces 3 - 10 - 12, 3 - 12 - 11, lead to the emergence of new flat faces, which need to be closed by new polyhedrons, and this process is difficult to complete. Make it fails. It should be recognized that the assumption made at the beginning about the anti - cube - octahedron as a ligand polytope of compounds $Ru_3(CO)_{12}, Os_3(CO)_{12}$ is not correct, since it is not provable.

To create a geometric image of a cluster with the skeleton of a three - bar metal cycle, one should turn to the coordination of ligands around each atom of the cycle. This coordination is octahedral. In the case of a closed cycle, coordination around each atom overlaps each other. Consider the plane in which the metal cycle is located (Figure 12).

Figure 12. A section of a cluster containing a closed three - bar metal cycle



In this plane, there are three intersecting cross sections of the octahedron coordination of ligands around each metal atom. In the figures in Figure 12, these sections are:

1 - 2 - 4 - 5, 4 - 7 - 8 - 9, 5 - 7 - 13 – 14

Valence bonds are indicated by red edges. At the vertices 4, 5, 7 are located the metal atoms. In other vertices are located functional groups. Passing from the octahedron section into space, one should draw segments perpendicular to the section plane at vertices 4, 5, 7. These segments should intersect the section plane and are located above the section plane for the bond length and below the section plane for the bond length too. From the free vertices of these segments, the edges of the octahedrons connecting these vertices with the vertices of each corresponding octahedron should be drawn. The overall picture of the intersection of three octahedrons in the projection on the plane will be quite complicated. In addition, to create a geometric image of the entire cluster in the form of a convex closed figure, it is necessary to fill the space between the octahedrons. Here, as well as in the previous chapter, it is necessary to remove part of the edges of octahedrons that have ceased to bear the function of creating a convex figure in the cluster image, and add the edges necessary to create a convex figure in the cluster image. The final cluster figure is shown in Figure 13.

The vertices of the octahedrons above the sectional plane (Figure 12) are marked with numbers 3, 11, 15. The vertices of the octahedrons below the section plane (Figure 12) are designated with numbers 6, 10, 12. In accordance with what was said earlier, in Figure 13 eight edges of 6 - 5, 7 -9, 3 - 5, 7 - 11, 8 - 4, 2 - 4, 12 - 7, 1 - 5 from all edges of octahedrons with marked vertices are removed. At the same time, eight other edges are added 2 - 13, 8 - 14, 6 - 10, 10 - 12, 6 - 12, 3 - 15, 15 - 11, 3 - 11. The edges connecting the indicated vertices of three parallel octahedrons have blue color. The edges corresponding to the valence bonds are marked in red, the other edges have a black color. The construction in Figure 13 can be divided into two polytopes: one polytope, located above the section in which the closed cycle of metal atoms is located (Figure 14); another polytope is located under this section (Figure 15).

The section that separates both polytopes and at the same time belongs to both polytopes, taking into account the added and removed edges, has the form shown in Figure 16.

One defined the dimension of the upper part of the cluster shown in Figure 5. This part has 12 vertices ($f_0 = 12$), 35 edges ($f_1 = 35$):

1 - 2, 1 - 7, 1 - 3, 1 - 9, 2 - 3, 2 - 7, 2 - 13, 3 - 7, 3 - 4, 3 - 11, 3 - 13, 3 - 15, 4 - 7, 4 - 13, 4 - 15, 4 - 14, 4 - 11, 4 - 5, 5 - 11, 5 - 8, 5 - 9, 5 - 7, 5 - 14, 5 - 15, 7 - 13, 7 - 15, 8 - 11, 8 - 14, 8 - 9, 9 - 11, 11 - 14, 11 - 15, 13 - 14, 13 - 15, 14 - 15

41 two - dimensional elements ($f_2 = 41$):

1 - 2 - 7, 1 - 7 - 5 - 9, 1 - 7 - 3, 1 - 2 - 3, 1 - 3 - 11 - 9, 2 - 3 - 7, 2 - 3 - 13, 2 - 13 - 7, 3 - 13 - 15, 3 - 4 - 11, 3 - 4 - 15, 3 - 4 - 7, 3 - 7 - 15, 3 - 13 - 14 - 11, 3 - 13 - 4, 4 - 7 - 5, 4 - 5 - 11, 4 - 7 - 13, 4 - 5 - 14, 4 - 11 - 14, 3 - 13 - 7, 4 - 13 - 15, 4 - 11 - 15, 4 - 13 - 14, 4 - 15 - 14, 4 - 15 - 5, 4 - 7 - 15, 5 - 9 - 11, 5 - 15 - 11, 5 - 11 - 14, 5 - 14 - 8, 5 - 11 - 8, 5 - 15 - 14, 5 - 8 - 9, 8 - 11 - 14, 8 - 9 - 11, 11 - 15 - 14, 13 - 14 - 15, 3 - 7 - 4 - 15, 5 - 11 - 4 - 15, 3 - 7 - 5 - 11

18 three - dimensional elements ($f_3 = 18$):

1 - 2 - 7 - 3, 1 - 3 - 7 - 11 - 5 - 9, 2 - 3 - 7 - 13, 3 - 7 - 4 - 13, 3 - 7 - 4 - 15, 3 - 13 - 15 - 4, 3 - 13 - 15 - 14 - 11, 3 - 13 - 14 - 11 - 7 - 5, 3 - 4 - 11 - 14 - 13, 3 - 4 - 7 - 5 - 11, 4 - 7 - 5 - 15, 4 - 13 - 14 - 15, 4 - 5 - 11 - 14, 4 - 15 - 11 - 14, 5 - 15 - 11 - 14, 5 - 14 - 11 - 8, 5 - 11 - 8 - 14, 5 - 11 - 8 – 9

external three - dimensional surface of Figure 14.

Substituting the obtained values $f_i (i = 0, 1, 2, 3)$ in the equation (2) you can see that the Euler - Poincaré equation is satisfied in his case for $n = 4$:

$$12 - 35 + 41 - 18 = 0$$

This proves that Figure 14 is polytope with dimension 4.

The lower part of the cluster (Figure 15) is symmetrical to the upper part of the cluster (Figure 14) relative to the cross section separating them. The perpendiculars to the section 3-7, 5-11, 4-15 in the upper part of the cluster are equal in length to the perpendiculars to the section in the lower part of the cluster passing through the same points in the section, respectively, 7, 4, 5. Each edge in the upper part of the cluster has an edge in the lower part of the cluster. Therefore, the dimension of the polytope of the lower part of the cluster is equal to the dimension of the polytope of the upper part of the cluster, i.e. it is equal to 4. This can also be seen by directly counting the number of elements of different dimensions at the bottom of the cluster.

Figure 13. Spatial image of the cluster with a closed three - bar metal cycle

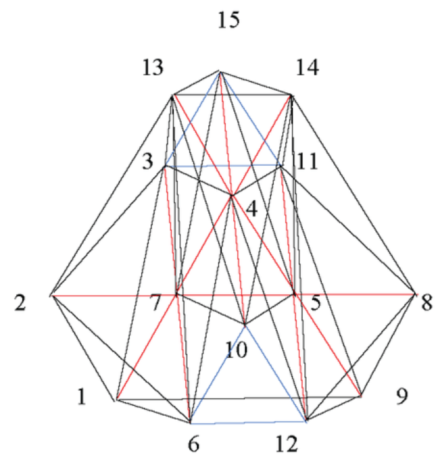


Figure 14. The polytope upper part of a cluster with a three - bar metal atom cycle

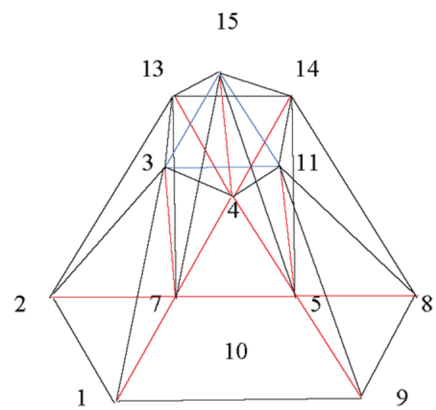


Figure 15. The polytope lower part of a cluster with a three - bar metal atom cycle

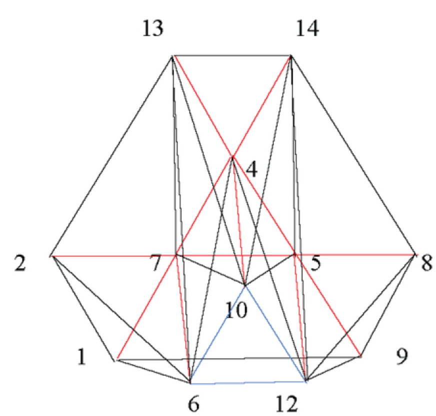
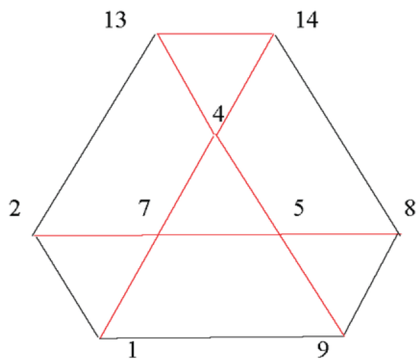


Figure 16. A section dividing a cluster with a three - bar closed cycle of metal atoms into two polytopes



Q.E.D.

The cluster ligand polyhedron is not an anti - cube - octahedron.

The top view of the cluster (from a point above the triangle 3 - 15 - 11) coincides with the view of the cluster from the bottom (from a point under triangle 6 - 10 - 12), as follows from Figure 17.

Only the numbers of the points of the blue triangle change (the numbers for the lower part of the cluster are indicated in brackets). The spatial image of the ligand polyhedron is shown in Figure 18.

As follows from Figures 8, 9 the ligand polyhedron contains 12 vertices ($f_0 = 12)$, 28 edges ($f_1 = 28)$, 18 flat faces (2 trapeziums, 16 triangles) ($f_2 = 18)$.

Substituting the obtained values $f_i (i = 0,1,2)$ in the equation (2) you can see that the Euler – Poincaré equation is satisfied in his case for $n = 3$:

$$12 - 28 + 18 = 2$$

This proves that Figure 18 is polyhedron with dimension 3.

It is clearly seen that the ligand polyhedron is not an anti - cube - octahedron, as was assumed earlier.

The ligand polyhedron cross section divides the ligand polyhedron into two parts, which are also three - dimensional surfaces. If the section is a hexagon, then in each half there are 9 vertices ($f_0 = 9)$, 17 edges ($f_1 = 17)$, 10 two - dimensional faces ($f_2 = 10)$. Substituting the obtained values $f_i (i = 0,1,2)$ in the equation (2) you can see that the Euler – Poincaré equation is satisfied in his case for $n = 3$:

$$9 - 17 + 10 = 2$$

If the cross section of the ligand polyhedron is the section in Figure 16 (it was used to analyze the upper and lower parts of the cluster when determining their dimensions), then each of the halves also represents a three - dimensional surface. In this case, for each of the halves, the number of vertices increases by 3, the number of edges increases by 9, the number of flat faces increases by 6. The total change in the right side of the Euler-Poincaré equation is $3 - 9 + 6 = 0$. Thus, the right side of equation (2) does not change. The surfaces remain three - dimensional.

Figure 17. Top and bottom views of ligand polyhedron

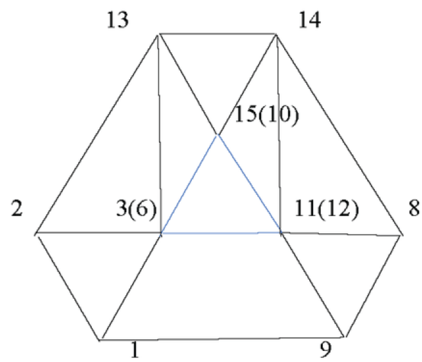
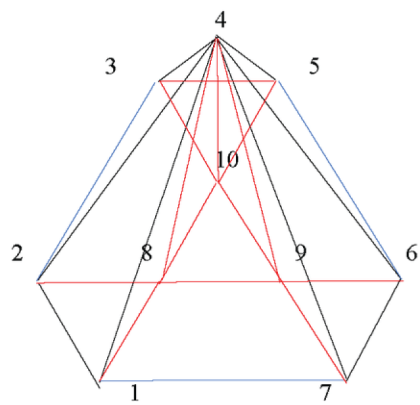


Figure 18. The spatial image of the ligand polyhedron



CONCLUSION

The geometry of multi-shell metal clusters with ligands is studied. It is proved that these clusters have the highest dimension and, depending on the geometry of the core (octahedron, cuboctahedron), the corresponding polytopes either have the type of cross-polytope, or their type differs significantly from the simplex and cross-polytope. It was shown that the core of giant palladium cluster containing 561 atoms with five shells has a dimension of 8. The erroneousness of the assertions that the core of giant palladium cluster is a lattice E_8 known in crystallography is proved. A spatial image of the cobalt tetra-anion cluster is presented and it is proved that its dimension is 5. The geometry of homo-element metal cycles with ligands is studied. In particular, it was proved that the ligands in the three nuclear carbonyls of ruthenium and osmium do not form a ligand polyhedron, as was previously assumed. The construction of cluster in this case can be divided into two polytopes: one polytope, located above the section in which the closed cycle of metal atoms is located; another polytope is located under this section.

Both polytopes adjacent to each other in a flat section have a dimension of 4.

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