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The Double Capping Phenomenon of Chemical Clusters

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Abstract The application of skeletal numbers has made it far much easier to categorize and analyze a wide range of clusters very quickly according to the 4N series method. It has been revealed that the clusters ranging from mono-to multi-skeletal elements comprise of two shells simply referred to as the inner (D) shell and the outer shell (C). A symbol to represent this duality concept has been introduced as the double capping parameter $K^* = C^yD^z$, where y+z = n, the number of skeletal elements in a cluster. Depending upon the cluster being analyzed, both C and could represent capping skeletal elements or in some cases, D could refer to capping electrons in dozen pairs. In other cases the C symbol could represent the missing skeletal elements for a cluster in order to achieve a CLOSO (fragment that follows S=4n+2 series) configuration. In order to demonstrate the double capping nature of clusters, about 40 clusters were categorized more than 30 of which were bi-metallic golden clusters. All of them were found to be capped with both C and D comprising of skeletal elements. The D elements are capped on the GENESIS ELECTRONS given by VE0=2z+2 electrons in the inner shell while the C elements are capped on top of the D closo elements. More examples of clusters were readily categorized into CLAN SERIES. A new equation for calculating the cluster valence electrons was derived as VE= 12y+14z+2 from $K^* = C^yD^z$. The calculated VE value was found to be the same as the one VF calculated directly from the cluster formula. The new equation for calculating cluster valence electrons is on of the six equations which can eaily be applied to calculate the cluster valence electrons of clusters and chemical elements of the periodic table except lanthanides and actinides.

Keywords Inner shell, Outer shell, Capping parameter, Double capping, Duality, Bi-metallic

1. Introduction

The unique shapes and intriguing nature of clusters have attracted a lot of scientists to the study of the same (Lipscomb, 1963; Wade, 1971, 1976, Mingos, 1972; Tolman, 1972; Rudolph, 1976; Pauling, 1977; Stone, 1981; Hoffmann, 1982; Teo, 1984; Hughes & Wade, 2000; Belyakova, 2003; Butcher, et al, 2003; Jemmis, 2005; Jemmis, etal, 2001a-b, 2002, 2003, 2008; Grimes, 2003; Goicoechea & Sevov, 2006; Fehlner & Halet, 2007; Mednikov & Dahl, 2010; Welch, 2013) for nearly fifty years. Relatively recently, an interest was ignited to understand the structural pattern of carbonyl clusters and this resulted into the development of a new approach to the categorization of clusters using the 4N series method out of which the skeletal numbers were discovered (Kiremire, 2016a-b; Kiremire, 2017a-e). The skeletal numbers have been found to be exceedingly fast and generally accurate in categorizing clusters and calculating the cluster valence electrons (Kiremire, 2018a-b). The structural prediction is also generally quite good (Kiremire, 2016c). The skeletal numbers have since been successfully applied to the analysis of a wide range of clusters including boranes, metalloboranes, metal carbonyls (Kiremire, 2017c), zintl, matryoshka (Kiremire, 2018c) clusters and the clusters of gold (Kiremire, 2018b). In this paper, the skeletal numbers will be applied to analyze the bimetallic clusters of gold and related clusters and the general features of clusters will be discussed.

2. Results and Discussion

Skeletal numbers

Skeletal numbers were assigned to all the elements of the periodic table except the lanthanides and actinides (Kiremire,

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2016a). Their derivation was based upon the valence electrons of the elements. Since main group and transition elements in the periodic table are arranged according to valence electrons, the skeletal numbers are also assigned to them according to their groups.

The range of the skeletal numbers is from K=7.5 to 0. This assignment is given in Table 1.

Table 1. Skeletal numbers of main group and transition metals

SN=K	V=2K	G	V+G	3d	4d	5d			
7.5	15	3	18	Sc	Y	Lu			
7.0	14	4	18	Ti	Zr	Hf			
6.5	13	5	18	V	Nb	Ta			
6.0	12	6	18	Cr	Mo	W			
5.5	11	7	18	Mn	Tc	Re			
5.0	10	8	18	Fe	Ru	Os			
4.5	9	9	19	Co	Rh	Ir			
4.0	8	10	18	Ni	Pd	Pt			
3.5	7	11	18	Cu	Ag	Au			
3.0	6	12	18	Zn	Cd	Hg			
				2s	3s	4s	5s	6s	7s
3.5	7	1	8	Li	Na	K	Rb	Cs	Fr
3.0	6	2	8	Be	Mg	Ca	Sr	Ba	Ra
2.5	5	3	8	B	Al	Ga	In	Tl	
2.0	4	4	8	C	Si	Ge	Sn	Ba	
1.5	3	5	8	N	P	As	Sb	Bi	
1.0	2	6	8	O	S	Se	Te	Po	
0.5	1	7	8	F	Cl	Br	I	At	
0.0	0	8	8	Ne	Ar	Kr	Xe	Rn	
SN=skeletal number, V=valence, G=group= valence electrons									

The skeletal number (K) of an element can be viewed as representing the number of electron pairs that element requires in order to attain the 8 or 18 electron rule for main group or transition elements respectively. Hence the valence V=2K represents the actual number of electrons needed by the respective element so as to attain a noble gas configuration.

THE VARIATION OF THE SKELETAL NUMBER

Let us consider what happens when we move from one skeletal element to the next one. This can be illustrated by considering the changes from Sc(K=7.5) to Zn(K=3) in the first row of transition metals. This is shown in Scheme 1,

$$Sc(7.5)+e\rightarrow Ti(7.0)+e\rightarrow V(6.5)+e\rightarrow Cr(6.0)+e\rightarrow Mn(5.5)+e\rightarrow Fe(5.0)\rightarrow Co(4.5)\rightarrow Ni(4.0)\rightarrow Cu(3.5)\rightarrow Zn(3.0)$$
$$Sc(7.5)+5e\equiv Sc^{5-}(K=5.0)\equiv Fe(5.0)$$

$$Fe(K=5)-5e = Fe^{5+}(K=7.5)\equiv Sc(K=7.5)$$

Scheme 1. Inter-conversion of skeletal elements

As can be seen, the addition of an electron to a skeletal element results into a reduction of a skeletal number of the element by 0.5 and hence a decrease in the skeletal valence (V=2K). Likewise, the removal of an electron from an element results into an increase in the skeletal number and a corresponding increase in the skeletal valence. This implies that an electron can be assigned a numerical value of -5, that is, e(K=-0,5) and similarly a positive charge (+1) can be assigned a numerical value of +0.5.

The variation of skeletal number can also be done by oxidizing the skeletal element. For instance, the carbon skeletal element C with a K value of 2, valence V=4, can be oxidized to C^{+} and then C^{2+} the K value changes from C(K=2, V=4)$\rightarrow C^{+}$(K=2.5, V=5) and C^{2+}(K=3, V=6). This variation of K value is reflected in the following golden carbon clusters (Gimeno, 2008)* shown in sketch Figure 1A.

$C + 4AuR = C(AuR)_4$
$C^+ + 5AuR = C(AuR)_5^+$
$C^{2+} + 6AuR = C(AuR)_6^{2+}$

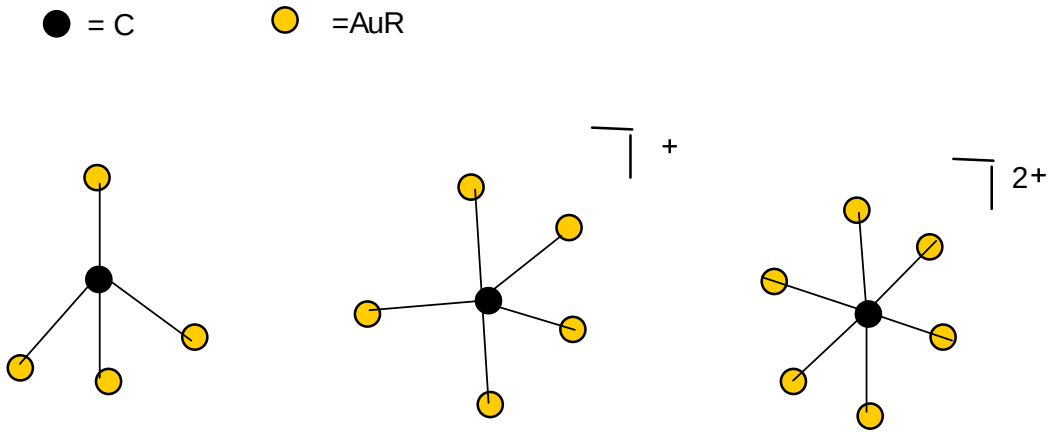


Figure 1A. The structures of $C(AuR)_4$, $C(AuR)_5^+$, and $C(AuR)_6^{2+}$

LIGANDS HAVE NEGATIVE SKELETAL NUMBERS

By analyzing cluster series, it was observed that addition of a CO ligand to a skeletal element results into a decrease of a cluster skeletal number (Kiremire, 2017c). The decrease is proportional to the number of electrons donated.

For instance, the hydrogen atom acting as a ligand donates one electron hence H(K= -0.5). The carbonyl ligand donates 2 electrons, CO(K= -1) for a cyclopentadienyl ligand C_5H_5(K= -2.5) and benzene, C_6H_6(K= -3).

CLUSTER NUMBER, K

A cluster with skeletal elements and ligands has a cluster number, K which can be regarded as a resultant contributions of the skeletal numbers of all the skeletal elements and the ligands in the cluster. If the cluster has no ligands, then the resultant K value will be derived from the constituent skeletal elements. This relationship can be expressed by the equation;

$$K = K_{SE} + K_L ,$$

Where K = cluster number, K_{SE} = contributions from the skeletal elements and K_L = contribution from the ligands.

DECOMPOSITION OF A CLUSTER FORMULA INTO A NUMERICAL NUMBER.

Since a cluster from the main group elements or transition metals comprises of skeletal elements and ligands, it can readily be decomposed into a simple numerical figure (K) which is generally a WHOLE NUMBER, This number can be utilized to generate cluster series S=4n+q, the skeletal number formula K=2n- ½ q where n is the number of skeletal elements in the cluster, and q is a variable which acts the determinant of the type of the cluster. Furthermore, the capping formula Kp= $C^yC[Mx]$, y+x=n, as well as double capping parameter implies there are two types of skeletal elements can be expressed by the formula $K^*=C^y+D^z$. The symbol y represents the capping elements of the cluster while x represents the number of nuclear elements of the cluster. The value z can be utilized to calculate the genesis cluster valence electrons (VE0=2z+2) of the series when n=0. With the knowledge of the series then, it is possible to derive the cluster valence electrons equation (Kiremire, 2018b) VEn=VE0+12n.

THE SKELETAL NUMBER K AS A STANDARDIZING PARAMETER OF THE SKELETAL ELEMENTS

The skeletal number can also be regarded to act as a standardizing parameter of cluster elements. Thus, all the skeletal elements can be considered to be equivalent and therefore can numerically be added. HOWEVER, THEIR CONTRIBUTIONS TO THE FINAL CLUSTER NUMBER (K) ARE NOT EQUIVALENT UNLESS IF THEY BELONG TO THE SAME PERIODIC GROUP.

THE DOUBLE CAPPING NATURE OF CHEMICAL CLUSTERS, $K^* = C^y + D^z$

The analysis of a wide range of clusters reveals that a cluster intrinsically comprises of two components given by $K^* = C^y + D^z$, where y and z are two separate entities related by y+z=n, the number of skeletal elements in a cluster. In a normal cluster y -represents the capping skeletal elements on top of z -nuclear CLOSO elements. The symbol z has a set of elements

which belong to the closo family, S=4n+2 while the capping elements, y obey a separate series given by S=4n-2y. The addition of the two equations yields the final overall cluster equation, S=(4n+2)+(4n-2y)=4n-2y+2. The double capping phenomenon can be illustrated by Figure 1B.

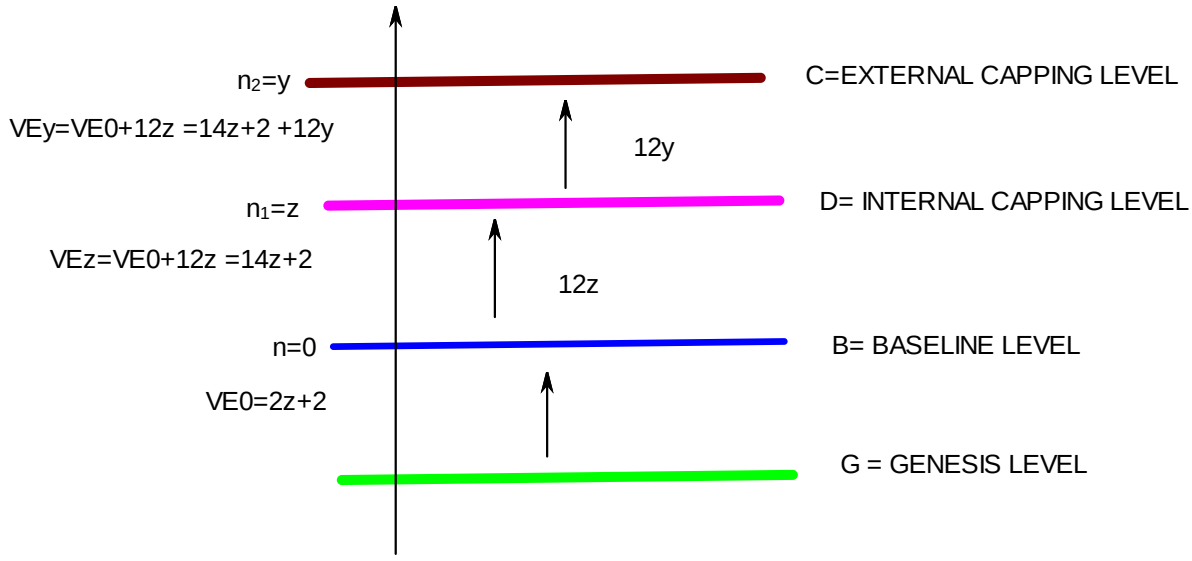


Figure 1B. Illustration of the capping phenomenon in clusters

D^6 ILLUSTRATIONS

We can illustrate the double capping nature of chemical clusters by taking the example of D^6 clan series. The D^6 represents an octahedral fragment with a K value of 11 and hence K(n)=11(6), and S=4n+2 (closo family). By analyzing the K(N) numerical series, it has been found that the transition metal clusters follow the 12N series while the main group element clusters follow the 2N series. But for now, let us focus on the 12N series for the D^6 system. As K decreases by 3 and n by 1, there is a corresponding decrease of cluster valence electrons by 12. Further step-wise decreases reaches a stage when n=0 (assigned to be the bottom-line). The corresponding cluster valence electrons(VE) is 14. Since VE0=14 for D^6 clan series, then the D^6 is related to VE0=14 by a simple equation VE0=2[6]+2 which is generalized to VE0=2z+2 for D^z clan trees (Kiremire, 2018b). The symbol VE0 is introduced to denote the cluster valence electrons when n= 0. A portion of D^6 clan tree series is given in Table 2. The table also gives one of the six formulas VE=18n-2K for calculating the cluster valence electrons, and the other five equations are given in Tables 3 and 4. These are:

VE=14n+q

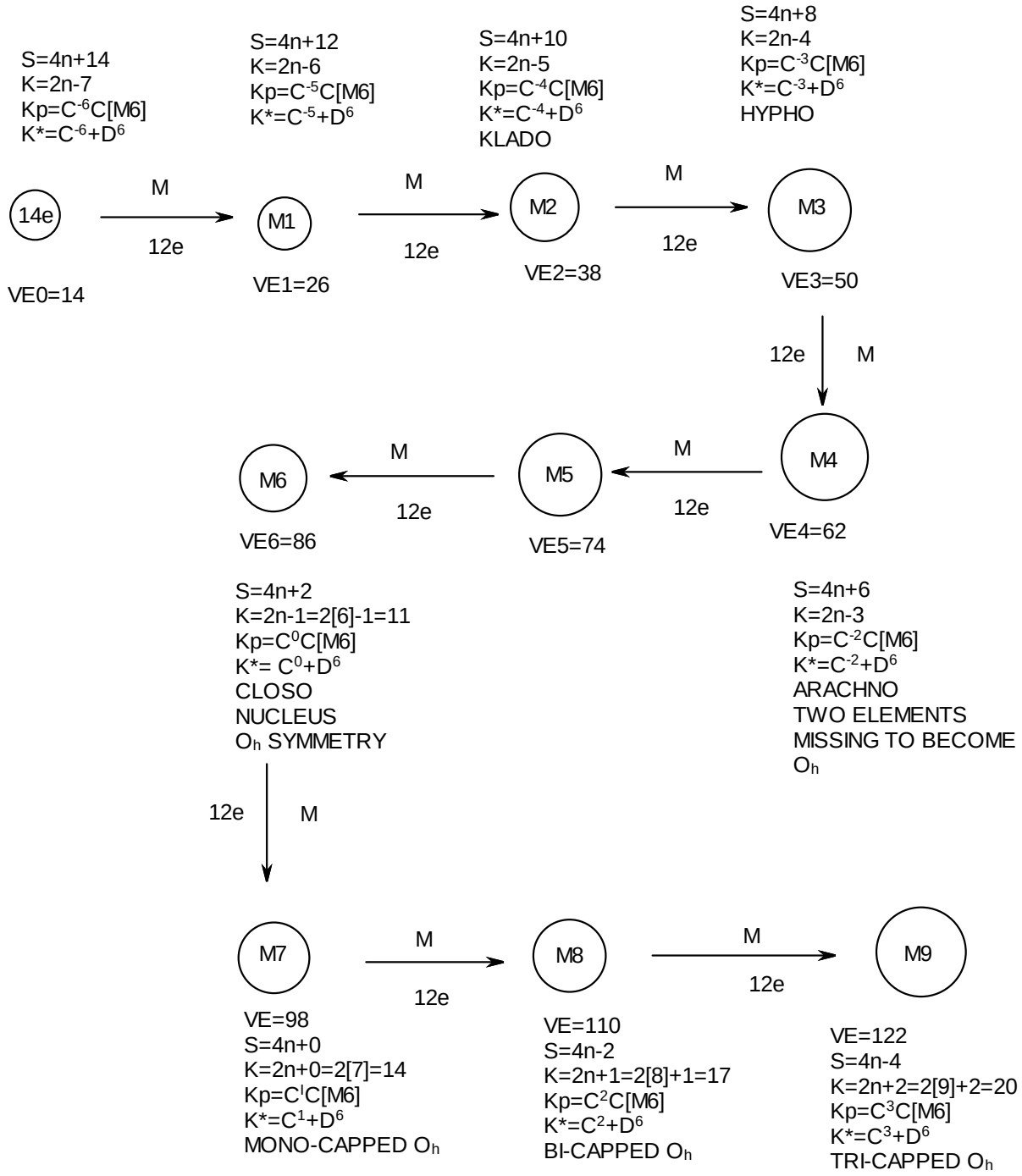
VE=VE0+12n [VE0=2z+2]

VE=VE0+12y+12z

VE=VEDz+12y [VEDz=14z+2]

VE=12y+14z+2

In addition, the table also gives the categorization series formula S=4n+q and cluster linkage formula K=2n- ½ q, the capping formula Kp= $C^yC[Mx]$ and the categorization formula K*= C^y+D^z. In 'conventional' clusters, y represents the number of capping elements and the z the number of elements in the cluster nucleus around which the capping elements form linkages. A selected number of known clusters which belong to D^6 cluster clan have also been included. As can be seen from Tables 2-4, the cluster valence electron series follow a smooth arithmetical progression which can be represented by T=a+12n, where T= cluster valence electrons, a= the number of cluster valence electrons when n=0 and n= the number of skeletal elements in a cluster. Since we are thinking of cluster valence electrons, the capping formula becomes VE=VE0+12n. Selected D^6 capping process is shown in Scheme 2. As can be seen from Scheme 2, there is some capping before the CLOSO level S=4n+2 is reached which can be expressed as K*= $C^{-y}+D^z$, whose base is VE0, in this case, VE0(n=0)=14 and the capping after the closo level, K*=C^y+D^z based on D^6 closo nucleus. The D^6 symbol represents an O_h fragment or a fragment with an ideal symmetry of $B_6H_6^{2-}$. Thus, there are two phases of capping processes, the one before the closo level and the other after the closo level. When y and z represent genuine skeletal elements, then D^z may be regarded as a cluster nucleus. THIS IS THE BASIS OF WHAT HAS BEEN TERMED AS THE DOUBLE CAPPING PHENOMENON OF CHEMICAL CLUSTERS. All chemical clusters that have been tested including single skeletal elements can be expressed as K*= C^y+D^z (where y or z can have positive or negative numerical values).



Scheme 2. An illustration of the D^6 capping process

Table 2. A Sample of the D^6 Clan Series

K	n	VE=	CAPPING SERIES	K=	Kp=	K*=	Examples
		18n-2K	S=4n+q	2n- ½ q	$C^yC[Mx]$	C^y+D^z	
-13	-2	-10	4n+18	2n-9	$C^{-8}C[M6]$	$C^{-8}+D^6$	
-10	-1	2	4n+16	2n-8	$C^{-7}C[M6]$	$C^{-7}+D^6$	
-7	0	14	4n+14	2n-7	$C^{-6}C[M6]$	$C^{-6}+D^6$	
-4	1	26	4n+12	2n-6	$C^{-5}C[M6]$	$C^{-5}+D^6$	
-1	2	38	4n+10	2n-5	$C^{-4}C[M6]$	$C^{-4}+D^6$	
2	3	50	4n+8	2n-4	$C^{-3}C[M6]$	$C^{-3}+D^6$	$Re_3H_2(CO)_{13}^{-1}$
5	4	62	4n+6	2n-3	$C^{-2}C[M6]$	$C^{-2}+D^6$	$Re_4(CO)_{16}^{2-}$
8	5	74	4n+4	2n-2	$C^{-1}C[M6]$	$C^{-1}+D^6$	$Re_5(C)(CO)_{16}(H)^{2-}$
11	6	86	4n+2	2n-1	$C^0C[M6]$	C^0+D^6	$Re_6(C)(CO)_{19}^{2-}$
14	7	98	4n+0	2n+0	$C^1C[M6]$	C^1+D^6	$Ru_6(B)(CO)_{17}(AuL)$
17	8	110	4n-2	2n+1	$C^2C[M6]$	C^2+D^6	$Ru_5Pt(C)(CO)_{15}(AuL)_2$
20	9	122	4n-4	2n+2	$C^3C[M6]$	C^3+D^6	$Ru_4Rh_2(B)(CO)_{15}(AuL)_3$
23	10	134	4n-6	2n+3	$C^4C[M6]$	C^4+D^6	$Co_6(C)(CO)_{12}(AuL)_4$
26	11	146	4n-8	2n+4	$C^5C[M6]$	C^5+D^6	$Os_9(CO)_{24}(AuL)_2$
29	12	158	4n-10	2n+5	$C^6C[M6]$	C^6+D^6	
32	13	170	4n-12	2n+6	$C^7C[M6]$	C^7+D^6	$Rh_{13}(CO)_{12}H_2^{3-}$
35	14	182	4n-14	2n+7	$C^8C[M6]$	C^8+D^6	
38	15	194	4n-16	2n+8	$C^9C[M6]$	C^9+D^6	
41	16	206	4n-18	2n+9	$C^{10}C[M6]$	$C^{10}+D^6$	
44	17	218	4n-20	2n+10	$C^{11}C[M6]$	$C^{11}+D^6$	
47	18	230	4n-22	2n+11	$C^{12}C[M6]$	$C^{12}+D^6$	
50	19	242	4n-24	2n+12	$C^{13}C[M6]$	$C^{13}+D^6$	
53	20	254	4n-26	2n+13	$C^{14}C[M6]$	$C^{14}+D^6$	$Pd_{16}Ni_4(CO)_{22}L_4^{2-}$
56	21	266	4n-28	2n+14	$C^{15}C[M6]$	$C^{15}+D^6$	
59	22	278	4n-30	2n+15	$C^{16}C[M6]$	$C^{16}+D^6$	$Pt_{19}(CO)_{24}(AuL)_3^{-1}$
62	23	290	4n-32	2n+16	$C^{17}C[M6]$	$C^{17}+D^6$	$Pd_{23}(CO)_{20}L_{10}$
65	24	302	4n-34	2n+17	$C^{18}C[M6]$	$C^{18}+D^6$	$Pt_{24}(CO)_{30}^{2-}$
68	25	314	4n-36	2n+18	$C^{19}C[M6]$	$C^{19}+D^6$	
71	26	326	4n-38	2n+19	**$C^{20}C[M6]$**	**$C^{20}+D^6$**	
74	27	338	4n-40	2n+20	**$C^{21}C[M6]$**	**$C^{21}+D^6$**	
77	28	350	4n-42	2n+21	**$C^{22}C[M6]$**	**$C^{22}+D^6$**	
80	29	362	4n-44	2n+22	**$C^{23}C[M6]$**	**$C^{23}+D^6$**	$Pd_{29}(CO)_{28}L_7^{2-}$
83	30	374	4n-46	2n+23	**$C^{24}C[M6]$**	**$C^{24}+D^6$**	$HPd_{30}(CO)_{26}L_{10}^{-1}$
86	31	386	4n-48	2n+24	**$C^{25}C[M6]$**	**$C^{25}+D^6$**	
89	32	398	4n-50	2n+25	**$C^{26}C[M6]$**	**$C^{26}+D^6$**	
92	33	410	4n-52	2n+26	**$C^{27}C[M6]$**	**$C^{27}+D^6$**	
95	34	422	4n-54	2n+27	**$C^{28}C[M6]$**	**$C^{28}+D^6$**	
98	35	434	4n-56	2n+28	**$C^{29}C[M6]$**	**$C^{29}+D^6$**	
101	36	446	4n-58	2n+29	**$C^{30}C[M6]$**	**$C^{30}+D^6$**	
104	37	458	4n-60	2n+30	**$C^{31}C[M6]$**	**$C^{31}+D^6$**	
107	38	470	4n-62	2n+31	**$C^{32}C[M6]$**	**$C^{32}+D^6$**	$Pt_{38}(CO)_{44}^{2-}$
110	39	482	4n-64	2n+32	**$C^{33}C[M6]$**	**$C^{33}+D^6$**	
113	40	494	4n-66	2n+33	**$C^{34}C[M6]$**	**$C^{34}+D^6$**	
116	41	506	4n-68	2n+34	**$C^{35}C[M6]$**	**$C^{35}+D^6$**	
119	42	518	4n-70	2n+35	**$C^{36}C[M6]$**	**$C^{36}+D^6$**	$Pd_{33}Ni_9(CO)_{41}L_6^{4-}$

122	43	530	4n-72	2n+36	**$C^{37}C[M6]$**	**$C^{37}+D^6$**	
125	44	542	4n-74	2n+37	**$C^{38}C[M6]$**	**$C^{38}+D^6$**	$Ni_{38}Pt_6(CO)_{48}(H)^{5-}$
128	45	554	4n-76	2n+38	**$C^{39}C[M6]$**	**$C^{39}+D^6$**	
131	46	566	4n-78	2n+39	**$C^{40}C[M6]$**	**$C^{40}+D^6$**	
134	47	578	4n-80	2n+40	**$C^{41}C[M6]$**	**$C^{41}+D^6$**	
137	48	590	4n-82	2n+41	**$C^{42}C[M6]$**	**$C^{42}+D^6$**	
140	49	602	4n-84	2n+42	**$C^{43}C[M6]$**	**$C^{43}+D^6$**	
143	50	614	4n-86	2n+43	**$C^{44}C[M6]$**	**$C^{44}+D^6$**	

Table 3. The D6 Clan Series showing the use of new equations for calculating cluster valence electrons

						z=6, VE0=2z+2=14
K	**N**	**VE=**	**CAPPING SERIES**	K*=	VE=	VE=
		18n-2K	**S=4n+q**	C^y+D^z	14n+q	VE0+12n
-13	**-2**	**-10**	**4n+18**	**$C^{-8}+D^6$**	**14[-2]+18=-10**	**14+12[-2]=-10**
-10	**-1**	**2**	**4n+16**	**$C^{-7}+D^6$**	**14[-1]+16=2**	**14+12[-1]=2**
-7	**0**	**14**	**4n+14**	**$C^{-6}+D^6$**	**14[0]+14=14**	**14+12[0]=14=GENESIS**
-4	**1**	**26**	**4n+12**	**$C^{-5}+D^6$**	**14[1]+12=26**	**14+12[1]=26**
-1	**2**	**38**	**4n+10**	**$C^{-4}+D^6$**	**14[2]+10=38**	**14+12[2]=38**
2	**3**	**50**	**4n+8**	**$C^{-3}+D^6$**	**14[3]+8=50**	**14+12[3]=50**
5	**4**	**62**	**4n+6**	**$C^{-2}+D^6$**	**14[4]+6=62**	**14+12[4]=62**
8	**5**	**74**	**4n+4**	**$C^{-1}+D^6$**	**14[5]+4=74**	**14+12[5]=74**
11	**6**	**86**	**4n+2**	**C^0+D^6**	**14[6]+2=86**	**14+12[6]=86**
14	7	98	4n+0	C^1+D^6	14[7]+0=98	14+12[7]=98
17	8	110	4n-2	C^2+D^6	14[8]-2-110	14+12[8]=110
20	9	122	4n-4	**C^3+D^6**	**14[9]-4=122**	**14+12[9]=122**
23	10	134	4n-6	**C^4+D^6**	**14[10]-6=134**	**14+12[10]=134**
26	11	146	4n-8	**C^5+D^6**	**14[11]-8=146**	**14+12[11]=146**
29	12	158	4n-10	**C^6+D^6**	**14[12]-10=158**	**14+12[12]=158**
32	13	170	4n-12	**C^7+D^6**	**14[13]-12=170**	**14+12[13]=170**
35	14	182	4n-14	**C^8+D^6**	**14[14]-14=182**	**14+12[14]=182**
38	15	194	4n-16	**C^9+D^6**	**14[15]-16=194**	**14+12[15]=194**
41	16	206	4n-18	**$C^{10}+D^6$**	**14[16]-18=206**	**14+12[16]=206**
44	17	218	4n-20	**$C^{11}+D^6$**	**14[17]-20=218**	**14+12[17]=218**
47	18	230	4n-22	**$C^{12}+D^6$**	**14[18]-22=230**	**14+12[18]=230**
50	19	242	4n-24	**$C^{13}+D^6$**	**14[19]-24=242**	**14+12[19]=242**
53	20	254	4n-26	**$C^{14}+D^6$**	**14[20]-26=254**	**14+12[20]=254**
56	21	266	4n-28	**$C^{15}+D^6$**	**14[21]-28=266**	**14+12[21]=266**
59	22	278	4n-30	**$C^{16}+D^6$**	**14[22]-30=278**	**14+12[22]=278**
62	23	290	4n-32	**$C^{17}+D^6$**	**14[23]-32=290**	**14+12[23]=290**
65	24	302	4n-34	**$C^{18}+D^6$**	**14[24]-34=302**	**14+12[24]=302**
68	25	314	4n-36	**$C^{19}+D^6$**	**14[25]-36=314**	**14+12[25]=314**
71	26	326	4n-38	**$C^{20}+D^6$**	**14[26]-38=326**	**14+12[26]=326**
74	27	338	4n-40	**$C^{21}+D^6$**	**14[27]-40=338**	**14+12[27]=338**
77	28	350	4n-42	**$C^{22}+D^6$**	**14[28]-42=350**	**14+12[28]=350**

Table 4. Demonstration of more equations for calculating cluster valence electrons using new equations

				Z=6	VE0=2z+2=14,12z=72	VEDz=14z+2=86	14z+2=86
K	**N**	**VE=**	**CAPPING SERIES**	K*=	VE=	VE=	VE=
		18N-2K	**S=4n+q**	C^y+D^z	VE0+12y+12z	VEDz+12y	12y+14z+2
-13	**-2**	**-10**	**4n+18**	**$C^{-8}+D^6$**	**14+12[-8]+12[6]=-10**	**86+12[-8]=-10**	**12[-8]+86=-10**
-10	**-1**	**2**	**4n+16**	**$C^{-7}+D^6$**	**14+12[-7]+12[6]=2**	**86+12[-7]=2**	**12[-7]+86=2**
-7	**0**	**14**	**4n+14**	**$C^{-6}+D^6$**	**14+12[-6]+12[6]=14**	**86+12[-6]=14**	**12[-6]+86=14**
-4	**1**	**26**	**4n+12**	**$C^{-5}+D^6$**	**14+12[-5]+72=26**	**86+12[-5]=26**	**12[-5]+86=26**
-1	**2**	**38**	**4n+10**	**$C^{-4}+D^6$**	**14+12[-4]+72=38**	**86+12[-4]=38**	**12[-4]+86=38**
2	**3**	**50**	**4n+8**	**$C^{-3}+D^6$**	**14+12[-3]+72=50**	**86+12[-3]=50**	**12[-3]+86=50**
5	**4**	**62**	**4n+6**	**$C^{-2}+D^6$**	**14+12[-2]+72=62**	**86+12[-2]=62**	**12[-2]+86=62**
8	**5**	**74**	**4n+4**	**$C^{-1}+D^6$**	**14+12[-1]+72=74**	**86+12[-1]=74**	**12[-1]+86=74**
11	**6**	**86**	**4n+2**	**C^0+D^6**	**14+12[0]+72=86**	**86+12[0]=86**	**12[0]+86=86**
14	7	98	4n+0	C^1+D^6	14+12[1]+72=98	**86+12[1]=98**	**12[1]+86=98**
17	8	110	4n-2	C^2+D^6	14+12[2]+72=110	**86+12[2]=110**	**12[2]+86=110**
20	9	122	4n-4	**C^3+D^6**	14+12[3]+72=122	**86+12[3]=122**	**12[3]+86=122**
23	10	134	4n-6	**C^4+D^6**	14+12[4]+72=134	**86+12[4]=134**	**12[4]+86=134**
26	11	146	4n-8	**C^5+D^6**	14+12[5]+72=146	**86+12[5]=146**	**12[5]+86=146**
29	12	158	4n-10	**C^6+D^6**	14+12[6]+72=158	**86+12[6]=158**	**12[6]+86=158**
32	13	170	4n-12	**C^7+D^6**	14+12[7]+72=170	**86+12[7]=170**	**12[7]+86=170**
35	14	182	4n-14	**C^8+D^6**	14+12[8]+72=182	**86+12[8]=182**	**12[8]+86=182**
38	15	194	4n-16	**C^9+D^6**	14+12[9]+72=194	**86+12[9]=194**	**12[9]+86=194**
41	16	206	4n-18	**$C^{10}+D^6$**	14+12[10]+72=206	**86+12[10]=206**	**12[10]+86=206**
44	17	218	4n-20	**$C^{11}+D^6$**	14+12[11]+72=218	**86+12[11]=218**	**12[11]+86=218**
47	18	230	4n-22	**$C^{12}+D^6$**	14+12[12]+72=230	**86+12[12]=230**	**12[12]+86=230**
50	19	242	4n-24	**$C^{13}+D^6$**	14+12[13]+72=242	**86+12[13]=242**	**12[13]+86=242**
53	20	254	4n-26	**$C^{14}+D^6$**	14+12[14]+72=254	**86+12[14]=254**	**12[14]+86=256**
56	21	266	4n-28	**$C^{15}+D^6$**	14+12[15]+72=266	**86+12[15]=266**	**12[15]+86=266**
59	22	278	4n-30	**$C^{16}+D^6$**	14+12[16]+72=278	**86+12[16]=278**	**12[16]+86=278**
62	23	290	4n-32	**$C^{17}+D^6$**	14+12[17]+72=290	**86+12[17]=290**	**12[17]+86=290**
65	24	302	4n-34	**$C^{18}+D^6$**	14+12[18]+72=302	**86+12[18]=302**	**12[18]+86=302**
68	25	314	4n-36	**$C^{19}+D^6$**	14+12[19]+72=314	**86+12[19]=314**	**12[19]+86=314**
71	26	326	4n-38	**$C^{20}+D^6$**	14+12[20]+72=326	**86+12[20]=326**	**12[20]+86=326**
74	27	338	4n-40	**$C^{21}+D^6$**	14+12[21]+72=338	**86+12[21]=338**	**12[21]+86=338**
77	28	350	4n-42	**$C^{22}+D^6$**	14+12[22]+72=350	**86+12[22]=350**	**12[22]+86=350**

3. Examples of Selected Clusters

Let us consider some selected examples including the bimetallic golden clusters (Ciabatti, 2015) to demonstrate the double capping nature of chemical clusters.

1. $Au_6L_6^{2+}$:K=6[3.5]-6[1]+2[0.5]=16,n=6
K(n)=16(6)
12-16=-4
S=4n-8
K=2n+4
Kp=C^5C[M1]
K*=C^5+D^1
D^1 represents capping of one skeletal element sitting on 4 genesis electrons given by VE0=2z+2=2[1]+2=4.
C^5 represents 5 skeletal elements capping upon D^1 element in the cluster nucleus.

VEn=VE0+12n=4+12[6]=76; cluster valence electrons based on capping theory.
VF=represents cluster valence electrons calculated from the cluster formula=6[11]+6[2]-2=76.

2. $Au_8L_7^{2+}$:K=8[3.5]-7[1]+2[0.5]=22,n=8
K(n)=22(8)
16-22=-6
S=4n-12
K=2n+6
Kp=C^7C[M1]
K*=C^7+D^1
VE0=2[1]+2=4
VEn=VE0+12n=4+12[8]=100
VF=8[11]+7[2]-2=100
One skeletal element surrounded by 7
other capping skeletal elements.
The cluster valence electrons from
theory, VEn=VF(from the cluster formula)

3. $Au_9L_8^{3+}$:K=9[3.5]-8[1]+3[0.5]=25,n=9
K(n)=25(9)
18-25=-7
S=4n-14
K=2n+7
Kp=C^8C[M1]
K*=C^8+D^1
VE0=2[1]+2=4
VEn=VE0+12n=4+12[9]=112
VF=9[11]+8[2]-3=112
One skeletal element surrounded by 8
other capping skeletal elements.
The cluster valence electrons from
theory, VEn=VF(from the cluster formula)

4. $Au_9L_5R_3$:K=9[3.5]-5[1]-3[0.5]=25,n=9
K(n)=25(9)
18-25=-7
S=4n-14
K=2n+7
Kp=C^8C[M1]
K*=C^8+D^1
VE0=2[1]+2=4
VEn=VE0+12n=4+12[9]=112
VF=9[11]+5[2]+3[1]=112
One skeletal element surrounded by 8
other capping skeletal elements.
The cluster valence electrons from
theory, VEn=VF(from the cluster formula)

5. $Os_5(C)(CO)_{14}(AuL)_2$:K=5[5]-1[2]-14[1]+2[3.5-1]=14
n=5+2=7
K(n)=14(7)
2[7]-14=0
S=4n+0
K=2n+0
Kp=C^1C[M6]
K*=C^1+D^6
A mono-capped octahedron.

VE0=2[6]+2=14
VEn=VE0+12n=14+12(7)=98
VF=5[8]+1[4]+14[2]+2[11+2]=98

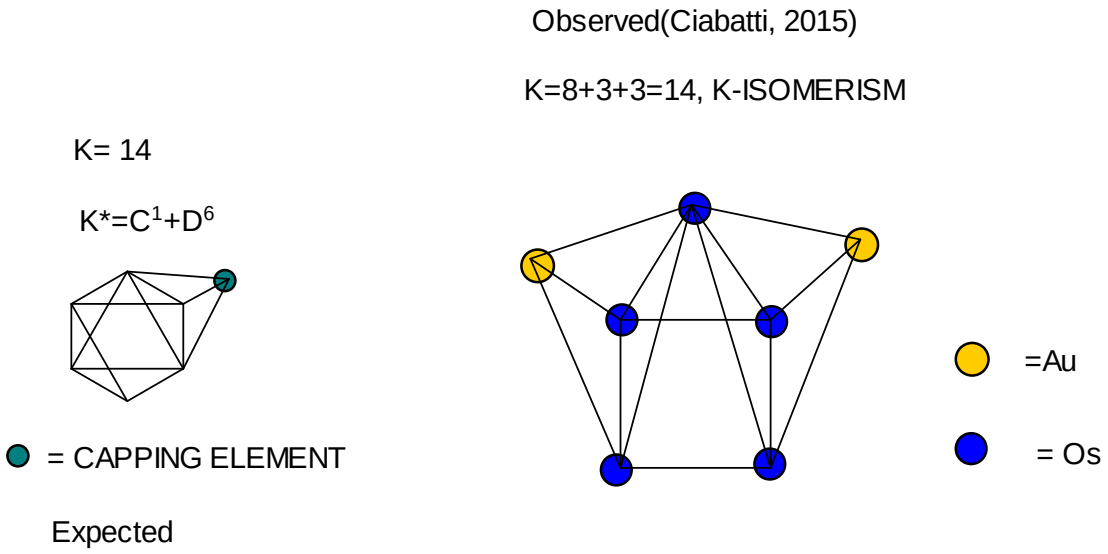


Figure 2. Isomeric graphical structure of $Os_5(C)(CO)_{14}(AuL)_2$

6. $Fe_5(C)(CO)_{14}(AuL)_2$:K=5[5]-1[2]-14[1]+2[3.5-1]=14
n=5+2=7
K(n)=14(7)
2[7]-14=0
S=4n+0
K=2n+0
Kp=C^1C[M6]
K*=C^1+D^6
A mono-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n=14+12(7)=98
VF=5[8]+1[4]+14[2]+2[11+2]=98

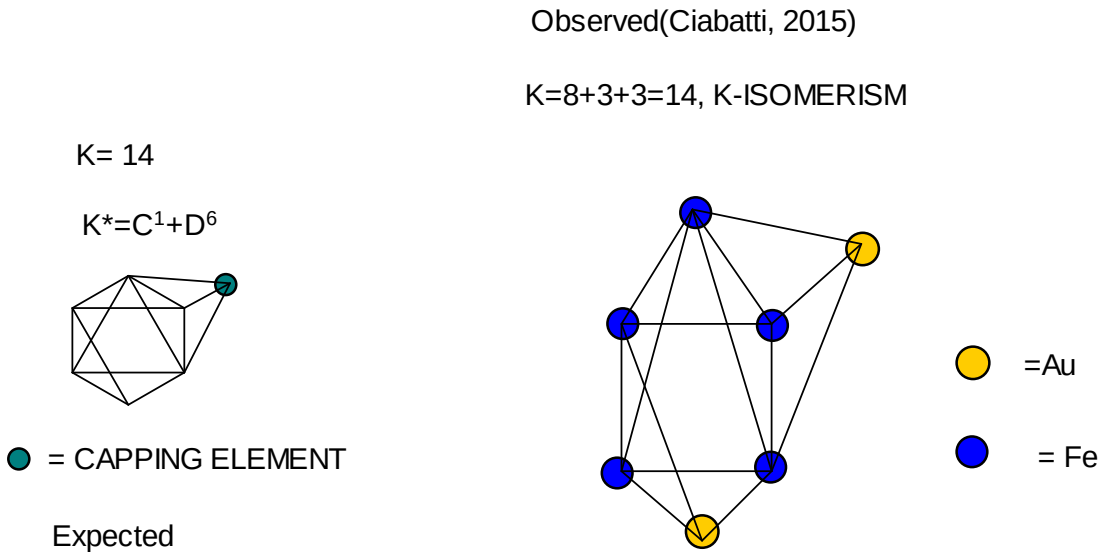


Figure 3. Isomeric graphical structure of $Fe_5(C)(CO)_{14}(AuL)_2$

7. $Ru_6(B)(CO)_{17}(AuL)$: K=6[5]-1[1.5]-17[1]+1[3.5-1]=14
n=6+1=7
K(n)=14(7)
2[7]-14=0
S=4n+0
K=2n+0
Kp=C^1C[M6]
K*=C^1+D^6
A mono-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[7]=98
VF=6[8]+1[3]+17[2]+1[11+2]=98

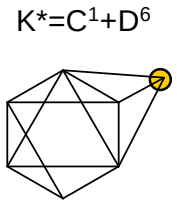


Figure 4. Predicted isomeric structure of $Ru_6(B)(CO)_{17}(AuL)$

The mono-capped octahedron shape is predicted and this is what is observed and the capping element is gold (Ciabatti, 2015).

8. $Co_5(C)(CO)_{11}(AuL)_2^{-1}$:K=5[4.5]+1[-2]+11[-1]+2[3.5-1]-1[0.5]=14
n=5+2=7
K(n)=14(7)
2[7]-14=0
S=4n+0
K=2n+0
Kp=C^1C[M6]
K* =C^1+D^6
VE0=2[6]+2=14
VEn=VE0+12n=14+12[7]=98
VF=5[9]+1[4]+11[2]+2[11+2]+1=98

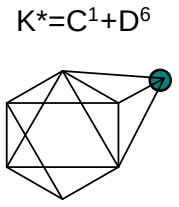


Figure 5. Predicted isomeric structure of $Co_5(C)(CO)_{11}(AuL)_2$

9. $Co_5(C)(CO)_{11}(AuL)_3$:K=5[4.5]-1[2]-11[1]+3[3.5-1]=17
n=5+3=8
K(n)=17(8)
2[8]-17=-1
S=4n-2
K=2n+1
Kp=C^2C[M6]
K*=C^2+D^6
A bi-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[8]=110
VF=5[9]+1[4]+11[2]+3[11+2]=110

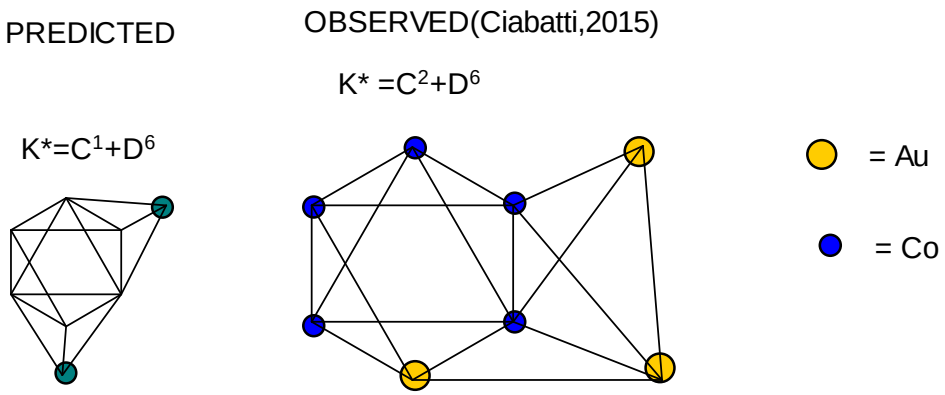


Figure 6. Isomeric graphical structure of $Co_5(C)(CO)_{11}(AuL)_3$

10. $Ru_6(C)(CO)_{16}(AuL)_2$:K=6[5]-1[2]-16[1]+2[3.5-1]=17
n=6+1=7
K(n)=17(8)
2[8]-17=-1
S=4n-2
K=2n+1
Kp=C^2C[M6]
K*=C^2+D^6
A bi-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n =14+12[8]=110
VF=6[8]+1[4]+16[2]+2[11+2]=110

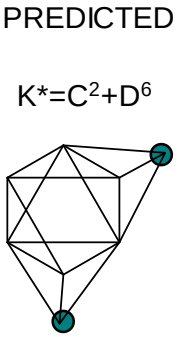


Figure 7. Predicted isomeric structure of $Ru_6(C)(CO)_{16}(AuL)_2$

11. $Fe_4Au_4(CO)_{16}^{4-}$:K=4[5]+4[3.5]-16[1]-4[0.5]=16
n=4+4=8
K(n)=16(8)
16-16=0
S=4n+0
K=2n+0
Kp=C^1C[M7] K*=C^1+D^7
VE0=2[7]+2=16
A mono-capped pentagonal bipyramid.
VEn=VE0+12n=16+12[8]=112
VF=4[8]+4[11]+16[2]+4=112

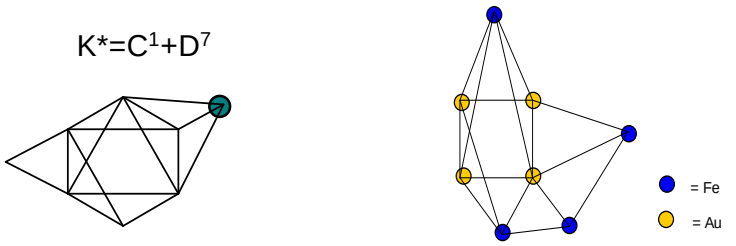


Figure 8. $Fe_4Au_4(CO)_{16}^{4-}$ Possible observed isomeric skeletal structure

Figure 8

12. $Ru_4Rh_2(B)(CO)_{15}(AuL)_3$:K=4[5]+2[4.5]-1[1.5]-15[1]+3[3.5-1]=20
n=4+2+3=9
K(n)=20(9)
2[9]-20=-2
S=4n-4
K=2n+2
Kp=C^3C[M6]
K*=C^3+D^6
A tri-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[9]=122
VF=4[8]+2[9]+1[3]+15[2]+3[11+2]=122

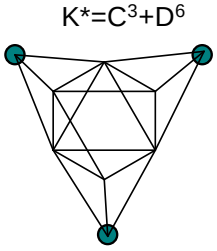


Figure 9. Predicted isomeric structure of $Ru_4Rh_2(B)(CO)_{15}(AuL)_3$

13. $Os_7(CO)_{20}(AuL)_2$: K=7[5]-20[1]+2[3.5-1=20
n=7+2=9
K(n)=20(9)
2[9]-20=-2
S=4n-4
K=2n+2
Kp=C^3C]M6]
K*=C^3+D^6
A tri-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+2n=14+12[9]=122
VF=7[8]+20[2]+2[11+2]=122

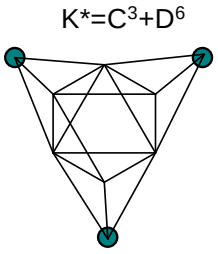


Figure 10. Predicted isomeric skeletal structure of $Os_7(CO)_{20}(AuL)_2$

14. $Fe_4Au_5(CO)_{16}^{3-}$:K=4[5]+5[3.5]-16[1]-3[0.5]=20
n=4+5=9
K(n)=20(9)
2[9]-20=-2
S=4n-4
K=2n+2
Kp=C^3C[M6]
K*=C^3+D^6
A tri-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[9]=122
VE=4[8]+5[11]]+16[2]+3=122

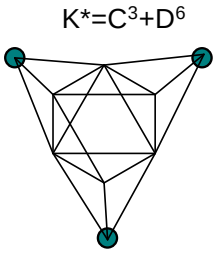


Figure 11. Predicted isomeric skeletal structure of $Fe_4Au_5(CO)_{16}^{3-}$

15. $Co_6(C)(CO)_{12}(AuL)_4$:K=6[4.5]-1[2]-12[1]+4[3.5-1]=23
n=6+4=10
K(n)=23(10)
2[10]-23=-3
S=4n-6
K=2n+3
Kp=C^4C[M6]
K*=C^4+D^6
A tetra-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[10]=134
VF=6[9]+1[4]+12[2]+4[11+2]=134

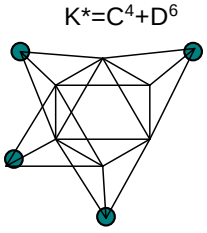


Figure 12. Predicted isomeric skeletal structure of $Co_6(C)(CO)_{12}(AuL)_4$

16. $Os_8(CO)_{22}(AuL)_2$: K=8[5]-22[1]+2[3.5-1]=23
n=8+2=10
K(n)=23(10)
2[10]-23=-3
S=4n-6
K=2n+3
Kp=C^4C[M6]
K*=C^4+D^6
A tetra-capped octahedron.
VE0=2[6]+2=14
VEn=VE0=14+12[10]=134
VF=8[8]+22[2]+2[11++2=134

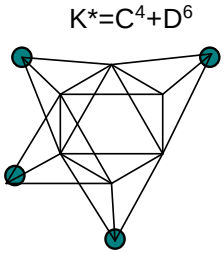
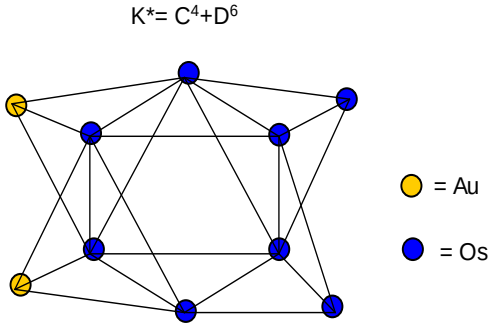


Figure 13. Predicted isomeric skeletal structure of $Os_8(CO)_{22}(AuL)_2$



Observed skeletal structure (Ciabatti, 2015)

17. $Ir_6Ru_3(CO)_{21}(AuL)^{-1}$:K=6[4.5]+3[5]-21[1]+1[3.5-1]-1[0.5]=23
n=6+3+1=10
K(n)=23(10)
2[10]-23=-3
S=4n-6
K=2n+3
Kp=C^4C[M6]
K*=C^4+D^6
A tetra-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[10]=134
VF=6[9]+3[8]+21[2]+1[11+2]+1=134

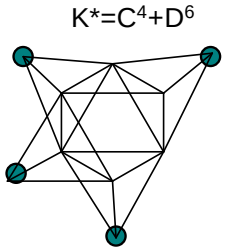


Figure 14. Predicted isomeric skeletal structure of $Ir_6Ru_3(CO)_{21}(AuL)^{-1}$

18. $Co_{10}(Au)(C)(CO)_{24}^{-1}$:K=10[4.5]+1[3.5]-1[2]-24[1]-1[0.5]=22
n=10+1=11
K(n)=22(11)
2[11]-22=0
S=4n+0
K=2n+0
Kp=C^1C[M10]
K*=C^1+D^{10}
A mono-capped bi-capped square-antiprism

VE0=2[10]+2=22
VEn=VE0+12n=22+12[11]=154
VF=10[9]+1[11]+1[4]+24[2]+1=154

19. $Os_9(CO)_{24}(AuL)_2$: K=9[5]-24[1]+2[3.5-1]=26
n=9+2=11
K(n)=26(11)
2[11]-26=-4
S=4n-8
K=2n+4
Kp=C^5C]M6]
K*=C^5+D^6
Penta-capped octahedron.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[11]=146
VF=9[8]+24[2]+2[11+2]=146

$K^*=C^5+D^6$

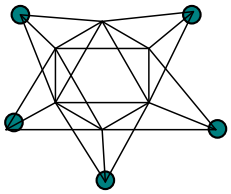


Figure 15. Predicted isomeric skeletal structure of $Os_9(CO)_{24}(AuL)_2$

20. $Ir_7Ru_3(CO)_{23}(AuL)^{-2}$:K=7[4.5]+3[5]-23[1]-2[0.5]=25
n=7+3+1=11
K(n)=25(11)
2[11]-25=-3
S=4n-6
K=2n+3
Kp=C^4C[M7]
K*=C^4+D^7
Tetra-capped pentagonal bipyramid.
VE0=2[7]+2=16
VEn=VE0+12n=16+12[11]=148
VF=7[9]+3[8]+23[2]+1[11+2]+2=148

$K^*=C^4+D^7$

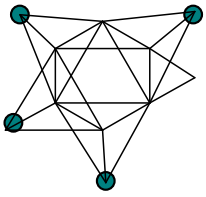


Figure 16. Predicted isomeric skeletal structure of $Ir_7Ru_3(CO)_{23}(AuL)^{-2}$

21. $Os_{10}(C)(CO)_{24}(AuL)^{-1}$:K=10[5]-1[2]-24[1]+1[3.5-1]-1[0.5]=26
n=10+1=11
K(n)=26(11)
2[11]-26=-4
S=4n-8
K=2n+4
Kp=C^5C[M6]
K*=C^5+D^6

Penta-capped octahedron
VE0=2[6]+2=14
VEn=VE0+12n=14+12[11]=146
VF=10[8]+1[4]+24[2]+1[11+2]+1=146

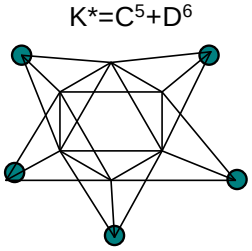


Figure 17. Predicted isomeric skeletal structure of $Os_{10}(C)(CO)_{24}(AuL)^{-1}$

22. $Co_{11}C_2(CO)_{23}^{-1}$:K=11[4.5]-2[2]-23[1]-1[0.5]=22
n=11
K(n)=22(11)
2[11]-22=0
S=4n+0
K=2n+0
Kp=C^1C[M10]
K*=C^1+D^{10}
Mono-capped bi-capped square-antprism
VE0=2[10]+2=22
VEn=VE0+12n=22+12[11]=154
VF=11[9]+2[4]+23[2]+1=154

23. $Os_8(CO)_{20}(AuL)_4$:K=8[5]-20[1]+4[3.5-1]=30
n=8+4=12
K(n)=30(12)
2[12]-30=-6
S=4n-12
K=2n+6
Kp=C^7[M5]
K*=C^7+D^5
Hepta-capped trigonal-bipyramid.
VE0=2[5]+2=12
VEn=VE0+12[12]=156
VF=8[8]+20[2]+4[13]=156

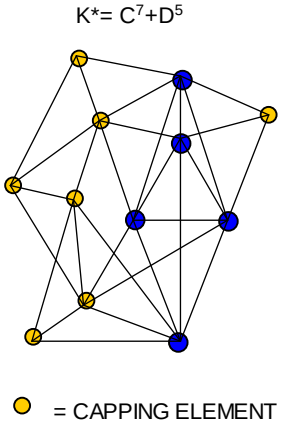


Figure 18. Predicted isomeric skeletal structure of $Os_8(CO)_{20}(AuL)_4$

24. $Rh_{12}(C_2)(CO)_{23}(AuL)^{-1}$:K=12[4.5]+2[-2]-23[1]+1[3.5-1]-1[0.5]=29
n=12+1=13
K(n)=29(13)
2[13]-29=-3
S=4n-6
K=2n+3
Kp=C4C[M9]
$K^*=C^4+D^9$
Penta-capped tri-capped trigonal prism.
VE0=2[9]+2=20
VEn=VE0+12n=20+12[13]=176
VF=12[9]+2[4]+23[2]+1[11+2]+1=176

25. $Os_{10}(CO)_{24}(AuL)_4$:K=10[5]-24[1]+4[3.5-1]=36
n=10+4=14
K(n)=36(14)
2[14]-36=-8
S=4n-16
K=2n+8
Kp=C^9C[M5]
$K^*=C^9+D^5$
Pentagonal bi-pyramd geometry surrounded by 9 capping skeletal elements.
VE0=2[5]+2=12
VEn=VE0+12n=12+12[14]=180
VF=10[8]+24[2]+4[13]=180

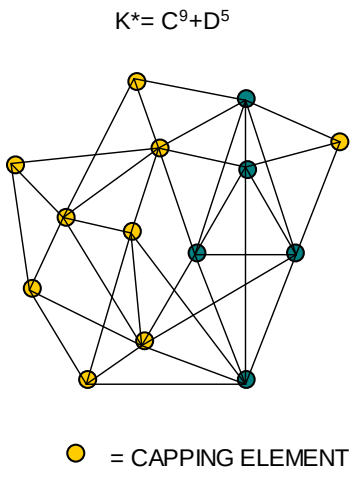
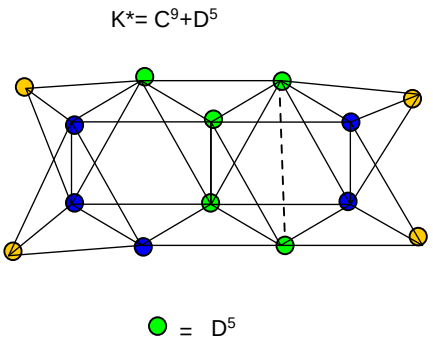


Figure 19. Predicted isomeric skeletal structure of $Os_{10}(CO)_{24}(AuL)_4$



26. $Ni_{12}Au_6(CO)_{24}^{2-}$: K=12[4]+6[3.5]-24-1=44,
n=12+6=18,
K(n)=44(18)
2[18]-44=-8
S=4n-16
K=2n+8
Kp=C^9C[M9]
K*=C^9+D^9
A tri-capped trigonal prism capped nine times.
K*=C^y+D^z
VE0=2z+2=2[9]+2=20
VEn=VE0+12n=20+12[18]=236
VF=12[10]+6[11]+24[2]+2=236

27. $Pt_{19}(CO)_{24}(AuL)_3^{-1}$:K=19[4]-24[1]+3[3.5-1]-1[0.5]=59
n=19+3=22
K(n)=59(22)
2[22]-59=-15
S=4n-30
K=2n+15
Kp=C^{16}C[M6]
K*=C^{16}+D^6
An octahedron capped 16 times.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[22]=278
VF=19[10]+24[2]+3[11+2]+1=278

28. $Fe_{10}Au_{21}(CO)_{40}^{5-}$:K=10[5]21[3.5]-40[1]-5[0.5]=81
n=10+21=31
K(n)=81(31)
2[31]-81=-19
S=4n-38
K+2n+19
Kp=C^{20}C[M11]
K*=C^{20}+D^{11}
An octadecahedron capped 20 times.
VE0=2[11]+2=24
VEn=VE0+12n=24+12[31]=396
VF=10[8]+21[11]+40[2]+5=396

29. $Pd_{28}Au_4(CO)_{22}L_{16}$:K=28[4]+4[3.5]-22[1]-16[1]=88
n=28+4=32
K(n)=88(32)
2[32]-88=-24
S=4n-48
K=2n+24
Kp=C^{25}C[M7]
K*=C^{25}+D^7
A pentagonal bipyramid capped 25 times.
VE0=2[7]+2=16
VEn=VE0+12n=16+12(32)=400
VF=28[10]+4[11]+22[2]+16[2]=400

30. $Fe_{12}Au_{22}(CO)_{48}^{6-}$:K=12[5]+22[3.5]-48[1]-6[0.5]=86
n=12+22=34
K(n)=86(34)
2[34]-86=-18

S=4n-36
K=2n+18
Kp=C^{19}C[M15]
K*=C^{19}+D^{15}
VE0=2z+2=2[15]+2=32
VEn=VE0+12n=32+12[34]=440
VF=12[8]+22[11]+48[2]+6=440

31. $Ni_{32}Au_6(CO)_{44}^{6-}$:K=32[4]+6[3.5]-44-3=106;
N=32+6=38
K(n)=106(38)
2[38]-106=-26
S=4n-52
K=2n+26
Kp=C^{27}C[M11]
K*=C^{27}+D^{11}
An octadecahedron capped 27 times.
VE0=2z+2=2[11]+2=24
VEn=VE0+12n=24+12[38]=480
VF=32[10]+6[11]+44[2]+6=480

32. $Fe_{14}Au_{28}(CO)_{52}^{8-}$: K=14[5]+28[3.5]-52[1]-8[0.5]=112
n=14+28=42
K(n)=112(42)
2[42]-112=-28
S=4n-56
K=2n+28
Kp=C29C[M13]
K*=C^{29}+D^{13}
A centered icosahedron capped 29 times.
VE0=2[13]+2=28
VEn=VE0+12n=28+12[42]=532
VF=14[8]+28[11]+52[2]+8=532

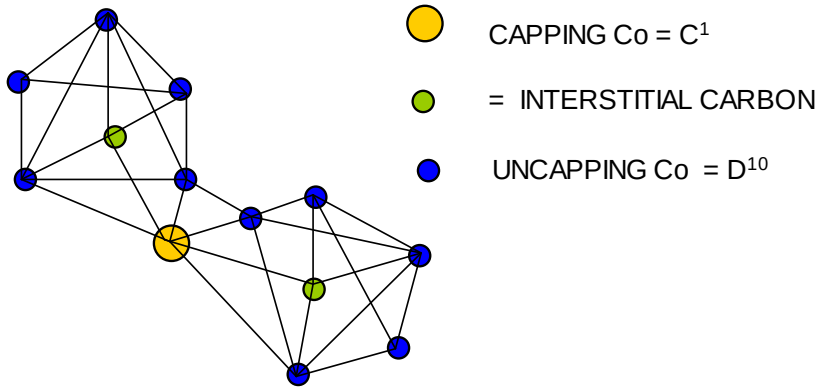
33. $Fe_{14}Au_{34}(CO)_{50}^{6-}$:K=14[5]+34[3.5]-50[1]-6[0.5]=136
n=14+34=48
K(n)=136(48)
2[48]-136=-40
S=4n-80
K=2n+40
Kp=C^{41}C[M7]
K*=C^{41}+D^{7}
A pentagonal bipyramid capped 41 times.
VE0=2[7]+2=16
VEn=VE0+12n=16+12[48]=592
VF=14[8]+34[11]+50[2]+6=592

34. $Co_{11}(C)_2(CO)_{23}^{-1}$:K=11[4.5]-2[2]-23[1]-1[0.5]=22,n=11
K(n)=22(11)
2[11]-22=0
S=4n+0
Kp=C^{1}C[M10]
K*=C^{1}+D^{10}
A mono-capped bi-capped square anti-prism.
VE0=2[z]+2=2[10]+2=22
VEn=VE0+12n=22+12[11]=154
VF=11[9]+2[4]+23[2]+1=154

The symbol $K^* = C^1+D^{10}$ predicts one skeletal element capping other 10 skeletal elements. This is shown in Figure 20 and is in agreement with what was reported (Ciabatti, 2015).

$Co_{11}C_2(CO)_{23}^{-1}$

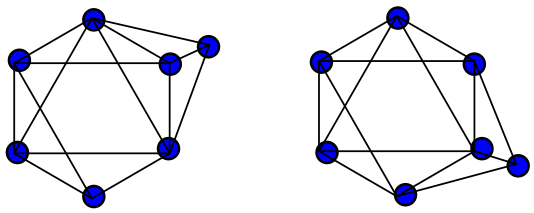
$K^* = C^1+D^{10}$



Observed someric structure of $Co_{11}C_2(CO)_{23}^{-1}$

Figure 20. Isomeric skeletal structure of $Co_{11}C_2(CO)_{23}^{-1}$

35. $Ru_6(B)(CO)_{17}(AuL)$:K=6[5]-1[1.5]-17(1)+1[3.5-1]=14
n=6+1=7
K(n)=14(7)
2[7]-14=0
S=4n+0
K=2n+0
$Kp=C^1C[M6]$
$K^*=C^1+D^6$; predicts a mono-capped octahedral symmetry. This is shown in F-2.
VE0=2[6]+2=14
VEn=VE0+12n=14+12[7]=98
VE=6[8]+1[3]+17[2]+1[11+2]=98



Predicted possible isomeric skeletal structures $Ru_6(B)(CO)_{17}(AuL)$

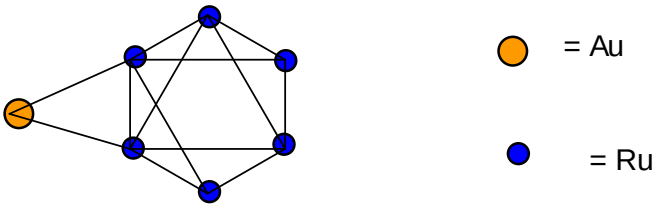


Figure 21. Observed isomeric structure of $Ru_6(B)(CO)_{17}(AuL)$

36. $Ir_6(B)(CO)_{14}(AuL)$:K =6[4.5]-1[1.5]-14[1]+1[3.5-1]=14
n=6+1=7
K(n)=14(7)
2[7]-14=0
S=4n+0
K=2n+0
Kp=C^1C[M6]
K*=C^1+D^6: predicts a mono-capped octahedral symmetry and this is observed (Ciabatti, 2015).
VE0=2[6]+2=14
VEn=14+12n=14+12[7]=98
VF=6[9]+1[3]+14[2]+1[11+2]=98

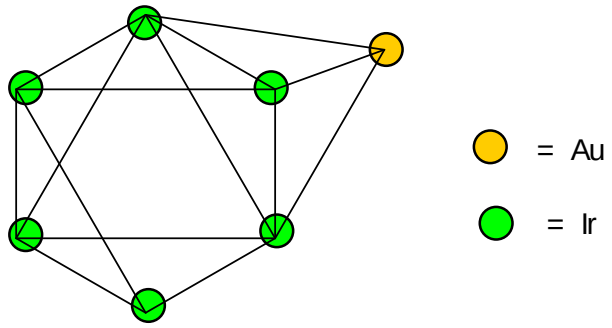
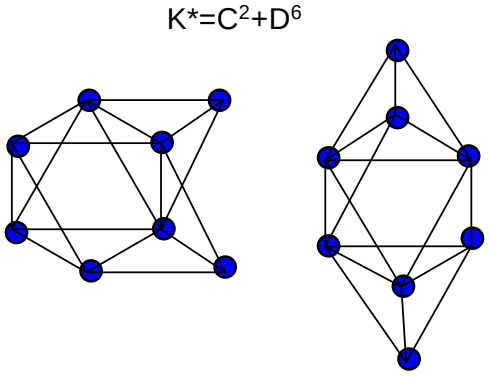


Figure 22. Observed isomeric skeletal structure of $Ir_6(B)(CO)_{14}(AuL)$

37. $Ru_5Pt(C)(CO)_{15}(AuL)_2$:K=5[5]+1[4]-1[2]-15[1]+2[3.5-1]=17
n=5+1+2=8
K(n)=17(8)
2[8]-17=-1
S=4n-2
K=2n+1
Kp=C^2C[M6]
K*=C^2+D^6; predicts a bi-capped octahedral symmetry and this is observed.**
VE0=2[6]+2=14
VEn=VE0+12n=14+12[8]=110
VF=5[8]+1[10]+1[4]+15[2]+2[11+1]=110



Possible predicted ideal isomeric skeletal structures of K*= C^2+D^6

The observed skeletal structure is given in Figure 23.

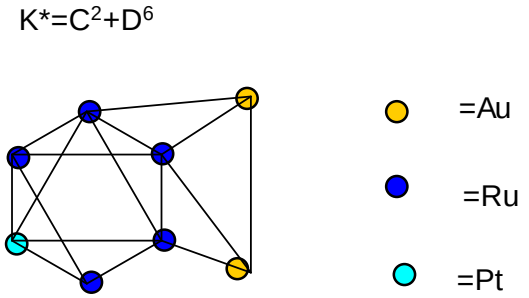


Figure 23. Observed isomeric skeletal structure of $Ru_5Pt(C)(CO)_{15}(AuL)_2$

38. $Ir_6(CO)_{15}(AuL)_2$:K=6[4.5]-15[1]+2[3.5-1]=17
n=6+2=8
K(n)=17(8)
2[8]-17=-1
S=4n-2
K=2n+1
Kp=C^2C[M6]
K*=C^2+D^6
VE0=2[6]+2=14
VEn=VE0+12n=14+12[8]=110
VF=6[9]+15[2]+2[11+2]=110

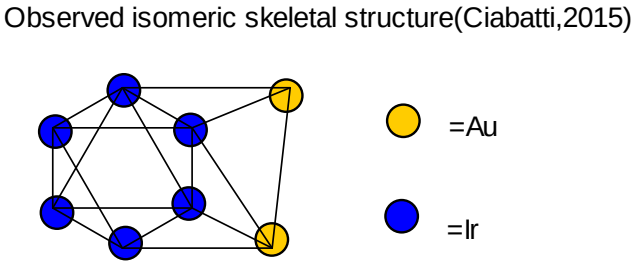


Figure 24. Isomeric skeletal $Ir_6(CO)_{15}(AuL)_2$

Other known isomeric skeletal bimetallic structures of gold are as shown below.

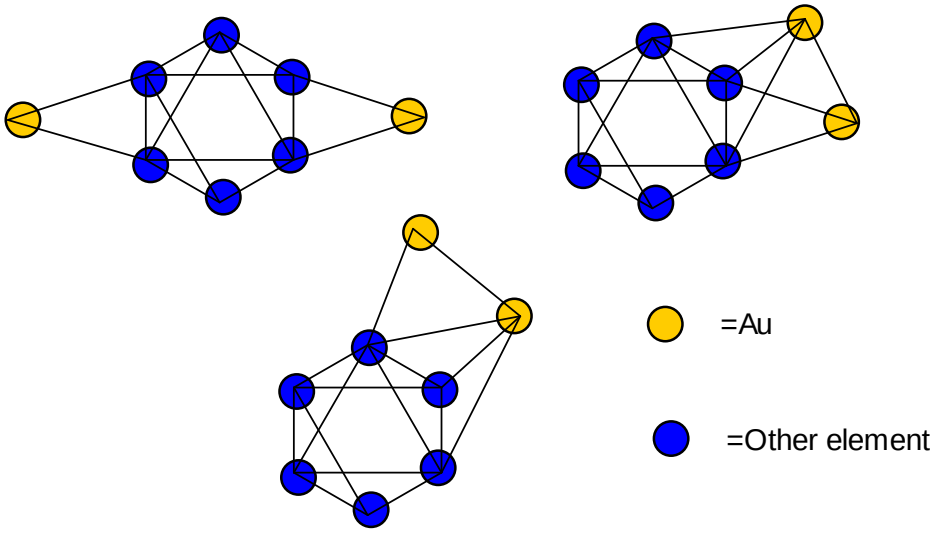
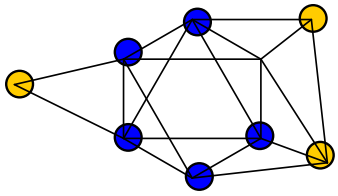


Figure 25. Other observed isomeric bimetallic skeletal structures of K* = C^2 + D^6

39. $Ru_4Rh_2(B)(CO)_{15}(AuL)_3$:K=4[5]+2[4.5]-1[1.5]-15[1]=20
n=4+2+3=9
K(n)=20(9)
2[9]-20=-2
S=4n-4
K=2n+2
Kp=$C^3C[M6]$
K*=C^3+D^6
VE0=2[6]+2=14
VEn=VE0+12n= 14+12[9]=122
VF=4[8]+2[9]+1[3]+15[2]+3[11+2]=122

Observed isomeric skeletal structure(Ciabatti,2015)



K* =C^3+D^6

Figure 26. Isomeric skeletal structure of $Ru_4Rh_2(B)(CO)_{15}(AuL)_3$

40. $Ru_6(B)(CO)_{16}(AuL)_3$:K=6[5]-1[1.5]-16[1]+3[3.5-1]=20
n=6+3=9
K(n)=20(9)
2[9]-20=-2
S=4n-4
K=2n+2
Kp=$C^3C[M6]$
K*=C^3+D^6
VE0=2[6]+2=14
VEn=VE0+12n=14+12[9]=122
VF=6[8]+1[3]+16[2]+3[11+2]=122

The observed isomeric skeletal strucure is shown below(Ciabatti,2015).

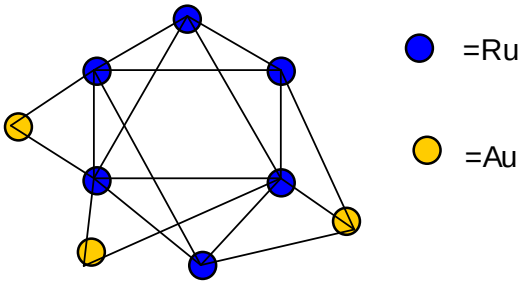
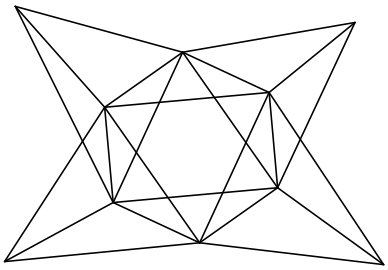


Figure 27. Isomeric skeletal structure of $Ru_6(B)(CO)_{16}(AuL)_3$

41. $Co_6(C)(CO)_{12}(AuL)_4$:K=6[4.5]-1[2]-12[1]+4[3.5-1]=23
n=6+4=10
K(n)=23(10)
2[10]-23=-3
S=4n-6
K=2n+3
Kp=C^4C[M6]
K*=C^4+D^6
VE0=2[6]+2=14
VEn=VE0+12n=14+12[10]=134
VEn=6[9]+1[4]+12[2]+4[11+2]=134



A possible isomeric skeletal symmetry for the cluster K* =C^4+D^6

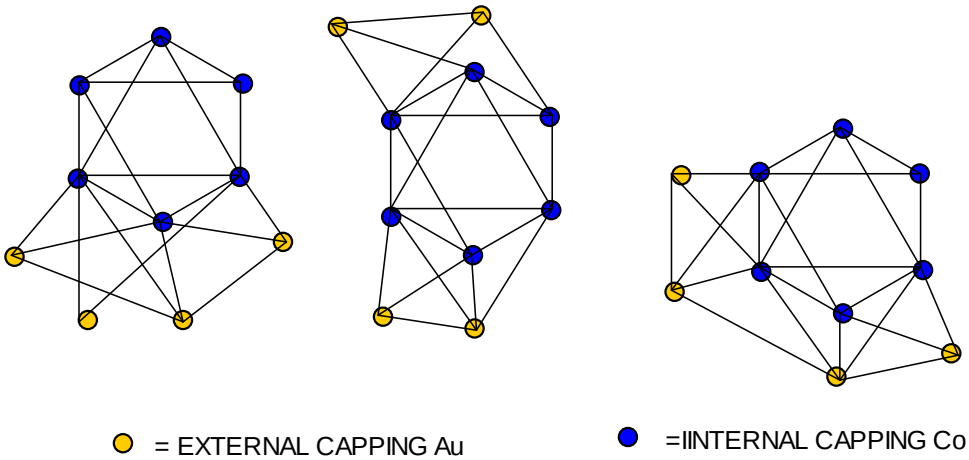
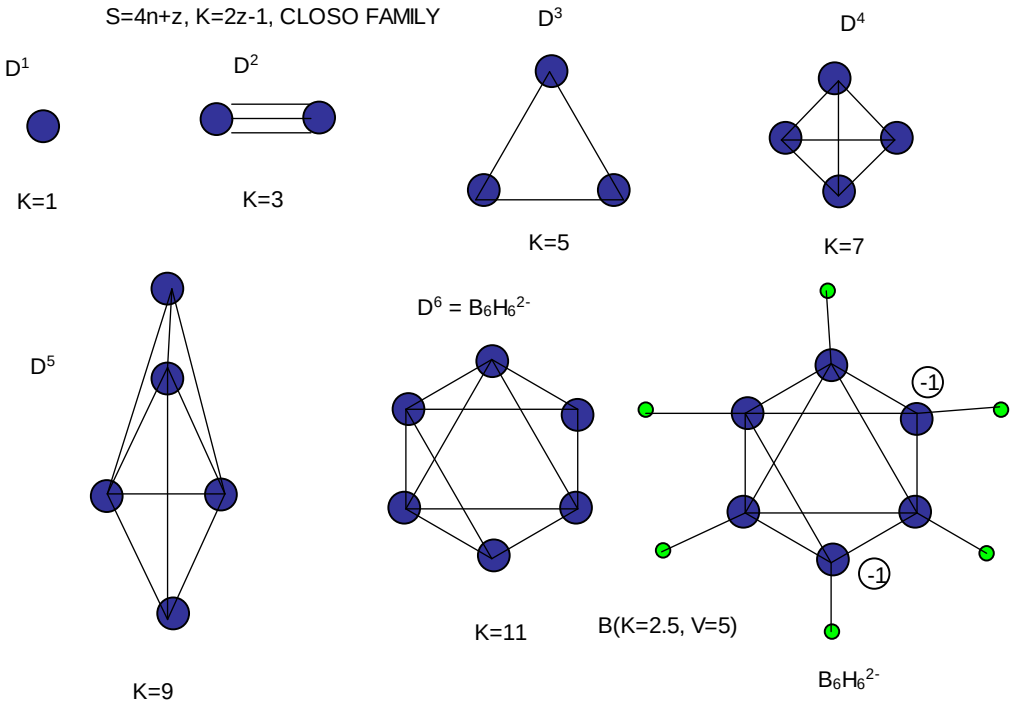


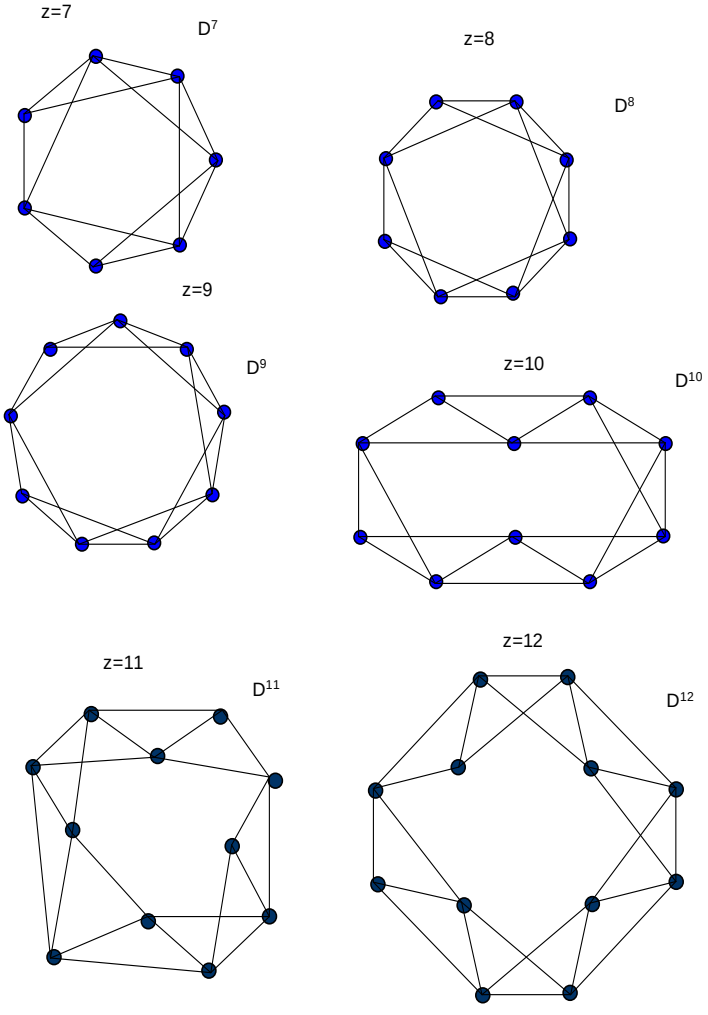
Figure 28. Observed isomeric skeletal structures of $Co_6(C)(CO)_{12}(AuL)_4$, L = PPh_3

The Concept of a Cluster Nucleus and the Double Capping Phenomenon K* = C^y+D^z

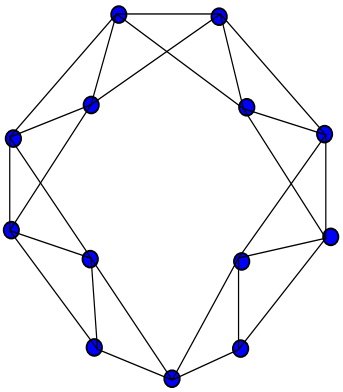
A wide range of bi-metallic gold clusters have been analyzed and categorized

As indicated above, 41 examples have been worked out using skeletal numbers. The categorization parameters K* derived from the calculations using skeletal numbers are provided as illustrations. The clusters have been organized according to the increasing magnitude of the clan parameter D^z, that is, increasing magnitude of z index. The results are summarized in Table 5. The categorization parameter is very useful as the number of skeletal elements involved can be derived, as well as their cluster clan, the series equation and the cluster valence electrons VE can also be calculated. In addition, the cluster geometry can tentatively be predicted. This information is also summarized in Table 5. The double capping nature of clusters is also reflected in Tables 5-6. The cluster clans range from D^1 to D^{20}. The matryoshka with K* =C^{13}+D^{20} (Huang, etal, 2014; King & Zhao, 2006) is a special case. The graphed hypothetical isomeric structures of selected D^z fragments (z=1-15 and 20) are given in Figure 29. According to the 4N series approach, the D^z fragments, in principle, correspond to the closo series $B_nH_n^{2-}$(n=1,2,3,4,5,6,7,8,9,etc). They represent the fundamental units around which clan series are based. In other words, they form the nuclei of clan clusters.


S=4n+z, K=2z-1, CLOSO FAMILY
D1
D2
D3
D4
K=1
K=3
K=5
K=7
D5
D6 = B6H6 2-
-1
-1
K=11
B(K=2.5, V=5)
K=9
B6H6 2-

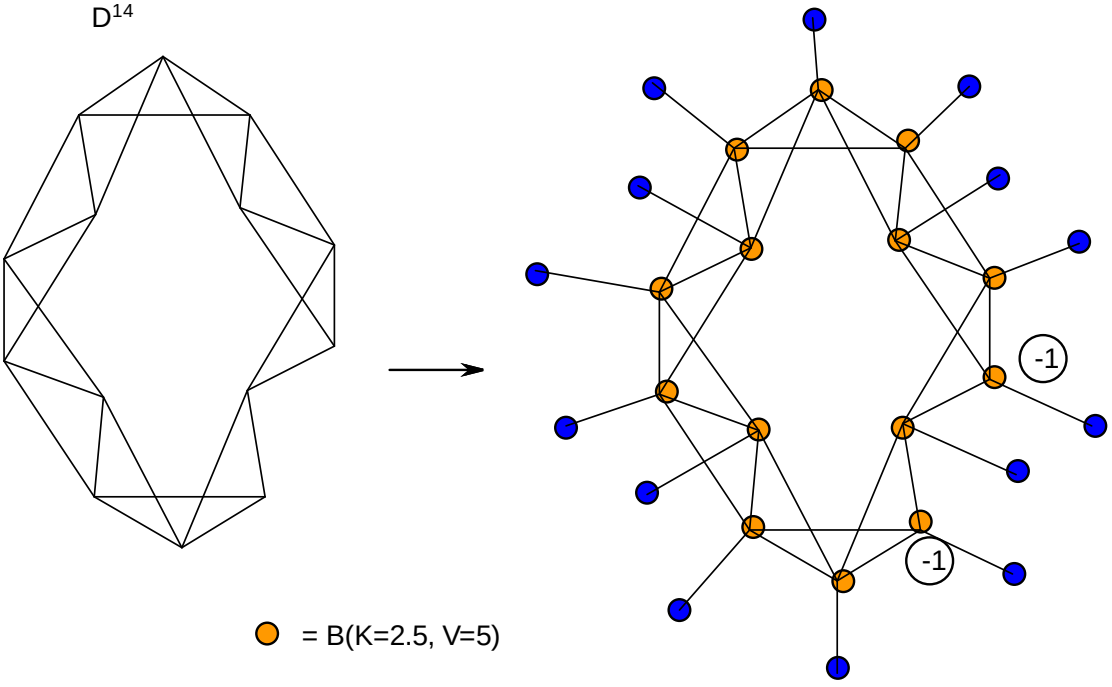

z=7
D7
z=8
D8
z=9
D9
z=10
D10
z=11
D11
z=12
D12

Z=13



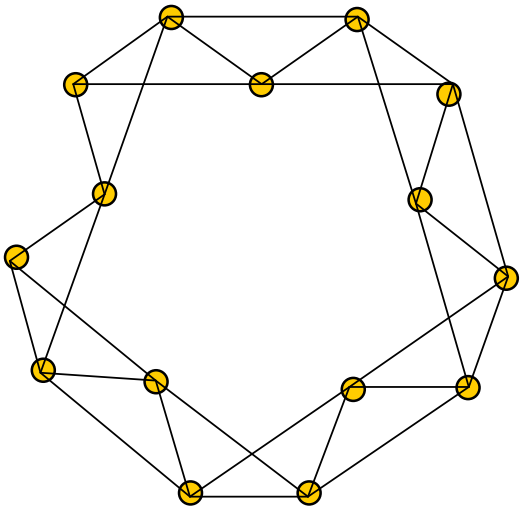
Isomeric graphical structures of D^z, z=1-13

D^{14}

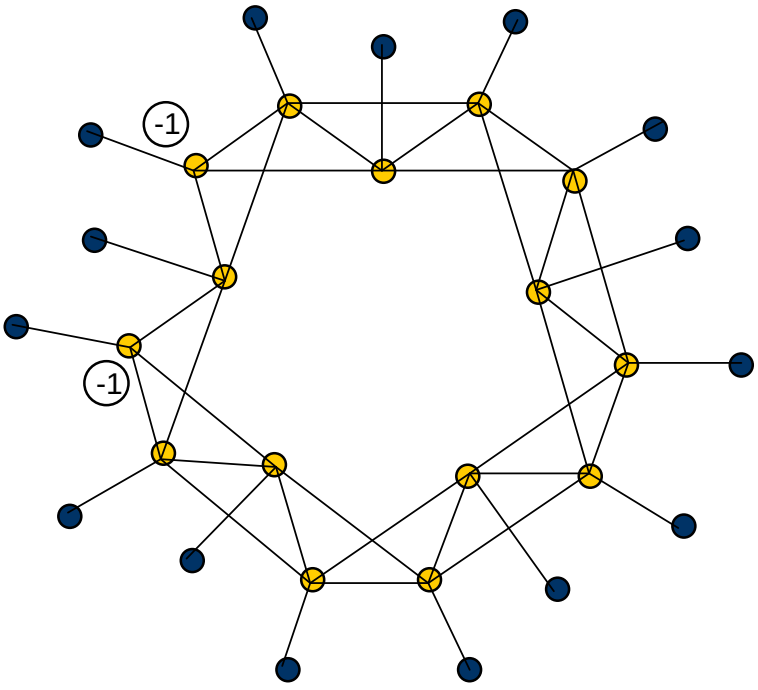


$D^{14} = B_{14}H_{14}^{2-}$

Isomeric graphical structure of D^{14}



= B(K=2.5, V= 5) = H(K= 0.5, V= 1)



Isomeric graphical structure of $D^{15}[B_{15}H_{15}^{2-}]$

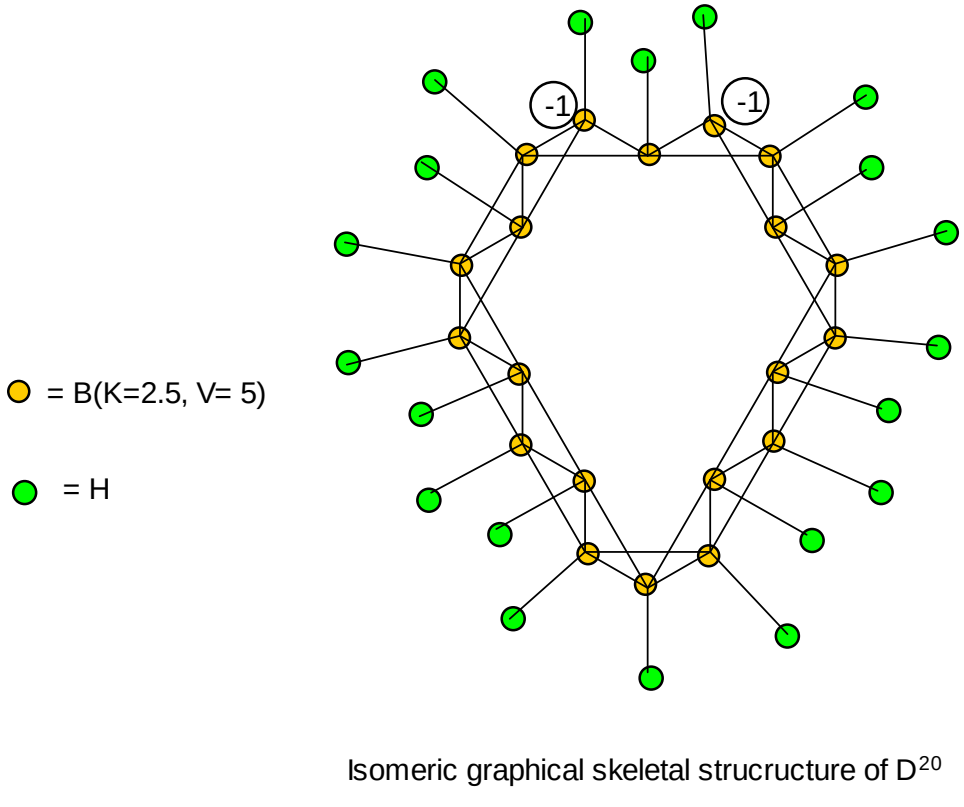


Figure 29. Isomeric graphical structures D^{1}-D^{15} and D^{20}

BRIEF SUMMARY OF THE ANALYSIS OF THE CATEGORIZED CLUSTERS

All the thirty-five bimetallic golden clusters with nuclearity index ranging from 7-42 analyzed were capped capping index ranging from C^{1} to C^{29}. It was found earlier that golden clusters have a have great tendency towards capping usually centered around D^{1} or D^{2} nucleus (Kiremire, 2017f, 2018d). This capping tendency appears to be portrayed in the bimetallic golden clusters as well. The predicted or observed isomeric skeletal structures of selected clusters are given in Figures 2-28. The nuclearity index in the capping bimetallic golden clusters ranged from D^{5}-D^{15}. These results are given in Table 5. According to the 4N series approach, the D^{z} fragments form the nuclei of the clusters. Selected isomeric graphical skeletal structures of D^{z}, z=1-15 and z=20 are shown in Figure 29. The formation of clusters can be viewed as a process of adding unitary fragments on to an appropriate CLUSTER VELENCE GENESIS ELECTRONS VE0=2z+2. For instance, z=1, VEO=4. This series will generate the D^{1} clan series, z=2, VE0=6, will give us the D^{2} clan series, z=3, VE0=8→D^{3} clan series, VEO=10→D^{4}, VE0=12→D^{5}, VEO=14→D^{6} series and so on. It has been observed that clusters or fragments with D^{z} where z<0, have metallic characteristics. This aspect has been covered mainly for a limited range transition metal clusters (Kiremire, 2018f). In this paper the concept has been applied to more than 200 clusters including many clusters from the main group elements and the skeletal elements of the periodic table excluding lanthanides (4f) and actinides (5f). This wide range of clusters are given in Table 6A. The clan series range from D^{-6} to D^{20} and the family series range from C^{-3} to C^{50}. The negative family capping index (C^{-y}) means that the cluster is below the CLOSO level whereas a positive capping index (C^{y}) means the cluster family is beyond the CLOSO level. Different cluster clans have been demarcated in the Table 6A with colored highlighters.

Table 5. Categorization of Selected Clusters and the Derivation of Cluster Valence Electrons from the Double Capping Parameter and Structure Prediction

T5	CLUSTER	K*=		VE=12y+12z+(2z+2)	OBSERVED	COMMENTS
		C^y+D^z	n	=12y+14z+2		
1	$Au_6L_6^{2+}$	C^5+D^1	6	12[5]+14[1]+2=76	76	One skeletal surrounded by 5 other capping elements
2	$Au_8L_7^{2+}$	C^7+D^1	8	12[7]+14[1]+2=100	100	One skeletal surrounded by 7 other capping elements
3	$Au_9L_8^{3+}$:	C^8+D^1	9	12[8]+16=112	112	One skeletal surrounded by 8 other capping elements
4	$Au_9L_5R_3$	C^8+D^1	9	12[8]+16=112	112	One skeletal surrounded by 8 other capping elements
23.	$Rh_{12}(C_2)(CO)_{23}(AuL)^{-1}$	C^7+D^5	12	7[12]+14[5]+2=156	156	Hepta-capped trigonal bipyramid
25.	$Os_{10}(CO)_{24}(AuL)_4$	C^9+D^5	14	9[12]+72=180	180	Trigonal bipyramid capped 9 times
35.	$Ru_6(B)(CO)_{17}(AuL)$	C^1+D^6	7	1[12]+86=98	98	Mono-capped octahedron
5	$Os_5(C)(CO)_{14}(AuL)_2$	C^1+D^6	7	12[1]+14[6]+2=98	98	Mono-capped octahedron
6	$Fe_5(C)(CO)_{14}(AuL)_2$	C^1+D^6	7	12[1]+86=98	98	Mono-capped octahedron
7.	$Ru_6(B)(CO)_{17}(AuL)$	C^1+D^6	7	12[1]+86=98	98	Mono-capped octahedron
8.	$Co_5(C)(CO)_{11}(AuL)_2^{-1}$	C^1+D^6	7	12[1]+86=98	98	Mono-capped octahedron
37.	$Ru_5Pt(C)(CO)_{15}(AuL)_2$	C^2+D^6	8	2[12]+86=110	110	Bi-capped octahedron
38.	$Ir_6(CO)_{15}(AuL)_2$	C^2+D^6	8	2[12]+86=110	110	Bi-capped octahedron
9.	$Co_5(C)(CO)_{11}(AuL)_3$	C^2+D^6	8	12[2]+86=110	110	Bi-capped octahedron
10.	$Ru_6(C)(CO)_{16}(AuL)_2$	C^2+D^6	8	12[2]+86=110	110	Bi-capped octahedron
39.	$Ru_6(B)(CO)_{16}(AuL)_3$	C^3+D^6	9	3[12]+86=122	122	Bi-capped octahedron
40.	$Ru_4Rh_2(B)(CO)_{15}(AuL)_3$	C^3+D^6	9	3[12]+86=122	122	tri-capped octahedron
12.	$Ru_4Rh_2(B)(CO)_{15}(AuL)_3$	C^3+D^6	9	3[12]+86=122	122	Tri-capped octahedron
13.	$Os_7(CO)_{20}(AuL)_2$	C^3+D^6	9	3[12]+86=122	122	Tri-capped octahedron
14.	$Fe_4Au_5(CO)_{16}^{3-}$	C^3+D^6	9	3[12]+86=122	122	Tri-capped octahedron
41.	$Co_6(C)(CO)_{12}(AuL)_4$	C^4+D^6	10	4[12]+86=134	134	tetra-capped octahedron
15.	$Co_6(C)(CO)_{12}(AuL)_4$	C^4+D^6	10	4[12]+86=134	134	Tetra-capped octahedron
16.	$Os_8(CO)_{22}(AuL)_2$	C^4+D^6	10	4[12]+86=134	134	Tetra-capped octahedron
17.	$Ir_6Ru_3(CO)_{21}(AuL)^{-1}$	C^4+D^6	10	4[12]+86=134	134	Tetra-capped octahedron
19.	$Os_9(CO)_{24}(AuL)_2$	C^5+D^6	11	5[12]+86=146	146	Penta-capped octahedron
21.	$Os_{10}(C)(CO)_{24}(AuL)^{-1}$	C^5+D^6	11	5[12]+86=146	146	Penta-capped octahedron
27.	$Pt_{19}(CO)_{24}(AuL)_3^{-1}$	$C^{16}+D^6$	22	16[12]+86=278	278	Octahedron capped 16 times
11.	$Fe_4Au_4(CO)_{16}^{4-}$:	C^1+D^7	8	1[12]+100=112	112	Mono-capped pentagonal bipyramid
20.	$Ir_7Ru_3(CO)_{23}(AuL)^{-2}$:	C^4+D^7	11	4[12]+100=148	148	tetra-capped $B_7H_7^{2-}$
29.	$Pd_{28}Au_4(CO)_{22}L_{16}$	$C^{25}+D^7$	32	25[12]+14[7]+2=400	400	$B_7H_7^{2-}$ capped 25 times
24.	$Rh_{12}(C_2)(CO)_{23}(AuL)^{-1}$	C^4+D^9	13	4[12]+14[9]+2=176	176	Tetra-capped $B_9H_9^{2-}$
26.	$Ni_{12}Au_6(CO)_{24}^{2-}$	C^9+D^9	18	9[12]+14[9]+2=236	236	$B_9H_9^{2-}$ capped 9 times
18.	$Co_{10}(Au)(C)(CO)_{24}^{-1}$	C^1+D^{10}	11	1[12]+142=154	154	Mono-capped $B_{10}H_{10}^{2-}$
34.	$Co_{11}(C)_2(CO)_{23}^{-1}$	C^1+D^{10}	11	1[12]+14[10]+2=154	154	$B_{10}H_{10}^{2-}$ mono-capped
36.	$Ir_6(B)(CO)_{14}(AuL)$	C^1+D^{10}	11	1[12]+14[10]+2=154	154	$B_{10}H_{10}^{2-}$ mono-capped
22.	$Co_{11}C_2(CO)_{23}^{-1}$	C^1+D^{10}	11	1[12]+142=154	154	Mono-capped $B_{10}H_{10}^{2-}$
28.	$Fe_{10}Au_{21}(CO)_{40}^{5-}$:	$C^{20}+D^{11}$	31	20[12]+14[11]+2=396	396	$B_{11}H_{11}^{2-}$ capped 20 times
31.	$Ni_{32}Au_6(CO)_{44}^{6-}$	$C^{27}+D^{11}$	38	27[12]+14[11]+2=480	480	$B_{11}H_{11}^{2-}$ capped 27 times
32.	$Fe_{14}Au_{28}(CO)_{52}^{8-}$	$C^{29}+D^{13}$	42	29[12]+14[13]+2=532	532	Centered icosahedron capped 29 times
33.	$Fe_{14}Au_{34}(CO)_{50}^{6-}$	$C^{29}+D^{13}$	42	29[12]+14[13]+2=532	532	Centered icosahedron capped 29 times
30.	$Fe_{12}Au_{22}(CO)_{48}^{6-}$	$C^{19}+D^{15}$	34	19[12]+14[15]+2=440	440	$B_{15}H_{15}^{2-}$ capped 19 times

Table 6A. Clusters arranged according to clan D (clan) series

						VE0=2z+2	VE=VE0+12n	VF
1	**$Pd_{42}Au_2(CO)_{26}L_{12}$**	**137(44)**	**4n-98**	**2n+49**	**$C^{50}+D^{-6}$**	**-10**	**518**	**518**
2	Sc, Y, Lu	7.5(1)	4n-11	2n+5.5	$C^{6.5}+D^{-5.5}$	-9	3	3
3	**Ti, Zr,Hf**	**7(1)**	**4n-10**	**2n+5**	**$C^{6}+D^{-5}$**	**-8**	**4**	**4**
4	$PdAu_{24}(SR)_{18}$	79(25)	4n-58	2n+29	$C^{30}+D^{-5}$	-8	292	292
5	V, Nb, Ta	6.5(1)	4n-9	2n+4.5	$C^{5.5}+D^{-4.5}$	-7	5	5
6	**Cr, Mo, W**	**6(1)**	**4n-8**	**2n+4**	**$C^{5}+D^{-4}$**	**-6**	**6**	**6**
7	Mn, Tc, Re	5.5(1)	4n-7	2n+3.5	$C^{4.5}+D^{-3.5}$	-5	7	7
8	**Fe, Ru,Os**	**5(1)**	**4n-6**	**2n+3**	**$C^{4}+D^{-3}$**	**-4**	**8**	**8**
9	$Pt_{12}AuL_{12}^{3+}$	41(13)	4n-30	2n+15	$C^{16}+D^{-3}$	-4	152	152
10	$Pt_{13}L_{12}^{2+}$	41(13)	4n-30	2n+15	$C^{16}+D^{-3}$	-4	152	152
11	Co, Rh, Ir	4.5(1)	4n-5	2n+2.5	$C^{3.5}+D^{-2.5}$	-3	9	9
12	$Os(CO)_1$	4(1)	4n-4	2n+2	$C^{3}+D^{-2}$	-2	10	10
13	**Ni, Pd,Pt**	**4(1)**	**4n-4**	**2n+2**	**$C^{3}+D^{-2}$**	**-2**	**10**	**10**
14	$Rh_8(CO)_9(C)$	25(8)	4n-18	2n+9	$C^{10}+D^{-2}$	-2	94	94
15	$Pt_{10}Au_3L_{12}^{3+}$	40(13)	4n-28	2n+14	$C^{15}+D^{-2}$	-2	154	154
16	$Pt_{11}Au_2L_{12}^{2+}$	40(13)	4n-28	2n+14	$C^{15}+D^{-2}$	-2	154	154
17	$Pd_{14}Tl_2(CO)_9L_4^{2+}$	49(16)	4n-34	2n+17	$C^{18}+D^{-2}$	-2	170	170
18	$Pd_{42}Au_2(CO)_{30}L_{12}$	133(44)	4n-90	2n+45	$C^{46}+D^{-2}$	-2	526	526
19	Cu,Ag, Au	3.5(1)	4n-3	2n+1.5	$C^{2.5}+D^{-1.5}$	-1	11	11
20	Li, Na, K, Rb, Cs	3.5(1)	4n-3	2n+1.5	$C^{2.5}+D^{-1.5}$	-1	1	1
21	**Be, Mg, Ca, Sr, Ba**	**3(1)**	**4n-2**	**2n+1**	**$C^{2}+D^{-1}$**	**0**	**2**	**2**
22	Zn, Cd, Hg	3(1)	4n-2	2n+1	$C^{2}+D^{-1}$	0	12	12
23	$Os(CO)_2$	3(1)	4n-2	2n+1	$C^{2}+D^{-1}$	0	12	12
24	$Pt_8Au_5L_{12}^{3+}$	39(13)	4n-26	2n+13	$C^{14}+D^{-1}$	0	156	170
25	$Pt_9Au_4L_{12}^{2+}$	39(13)	4n-26	2n+13	$C^{14}+D^{-1}$	0	156	156
26	B, Al, Ga,Tl, In	2.5(1)	4n-1	2n+0.5	$C^{1.5}+D^{-0.5}$	1	3	3
27	C, Si, Ge, Sn, Pb	2(1)	4n+0	2n+0	$C^{1}+D^{0}$	2	4	4
28	$Os(CO)_3$	2(1)	4n+0	2n+0	$C^{1}+D^{0}$	2	14	14
29	$Pt_6Au_7L_{12}^{3+}$	38(13)	4n-24	2n+12	$C^{13}+D^{0}$	2	158	158
30	$Pt_7Au_6L_{12}^{2+}$	38(13)	4n-24	2n+12	$C^{13}+D^{0}$	2	158	158
31	$Os_{20}(CO)_{40}^{2-}$	59(20)	4n-38	2n+19	$C^{20}+D^{0}$	2	242	242
32	**$Pd_{41}Au_2(CO)_{27}L_{16}$**	**128(43)**	**4n-84**	**2n+42**	**$C^{43}+D^{0}$**	**2**	**518**	**518**
33	N,P,As, Sb, Bi	1.5(1)	4n+1	2n-0.5	$C^{0.5}+D^{0.5}$	3	5	5
34	O, S,Se. Te	1(1)	4n+2	2n-1	$C^{0}+D^{1}$	4	6	6
35	$Os(CO)_4$	1(1)	4n+2	2n-1	$C^{0}+D^{1}$	4	16	16
36	**$RhClL_3$**	**1(1)**	**4n+2**	**2n-1**	**$C^{0}+D^{1}$**	**4**	**16**	**16**
37	AuL_3^{+1}	1(1)	4n+2	2n-1	$C^{0}+D^{1}$	4	16	16
38	$AuCl_4^{-1}$	1(1)	4n+2	2n-1	$C^{0}+D^{1}$	4	16	16
39	Au_2L_3	4(2)	4n+0	2n+0	$C^{1}+D^{1}$	4	28	28
40	$(AuL)_3IrL_2(NO_3)^{+1}$	10(4)	4n-4	2n+2	$C^{3}+D^{1}$	4	52	52
41	Au_5L_4Cl	13(5)	4n-6	2n+3	$C^{4}+D^{1}$	4	64	64
42	$Au_6L_4Cl_2$	16(6)	4n-8	2n+4	$C^{5}+D^{1}$	4	76	76
43	$Au_6L_6^{2+}$	16(6)	4n-8	2n+4	$C^{5}+D^{1}$	4	76	76
44	$Au_8L_7^{2+}$	21(8)	4n-12	2n+6	$C^{7}+D^{1}$	4	112	112
45	$Au_9L_8^{3+}$	24(9)	2n-14	2n+7	$C^{8}+D^{1}$	4	124	124
46	$Pt_6Au_6L_{12}^{2+}$	34(12)	4n-20	2n+10	$C^{9}+D^{1}$	4	148	148
47	$Pt_4Au_9L_{12}^{3+}$	37(13)	4n-22	2n+11	$C^{10}+D^{1}$	4	160	160
48	$Au_9L_{12}^{3+}$	37(13)	4n-22	2n+11	$C^{10}+D^{1}$	4	160	160

49	**$Pt_5Au_8L_{12}^{2+}$**	**37(13)**	**4n-22**	**2n+11**	**$C^{10}+D^1$**	**4**	**160**	**160**
50	F, Cl, Br, I	0.5(1)	4n+3	2n-1.5	$C^{-0.5}+D^{1.5}$	5	7	7
51	**BH_5**	**0(1)**	**4n+4**	**2n-2**	**$C^{-1}+D^2$**	**6**	**8**	**8**
51	Ne,Ar,Kr, Xe	0(1)	4n+4	2n-2	$C^{-1}+D^2$	6	8	8
53	B_2H_4	3(2)	4n+2	2n-1	C^0+D^2	6	10	10
54	**$Fe(CO)_5$**	**0(1)**	**4n+4**	**2n-2**	**$C^{-1}+D^2$**	**6**	**18**	**18**
55	$Os(CO)_5$	0(1)	4n+4	2n-2	$C^{-1}+D^2$	6	18	18
56	$IrH_3L_3(AuL)^{+1}$	3(2)	4n+2	2n-1	C^0+D^2	6	30	30
57	$(AuL)_2Fe(CO)_4$	6(3)	4n+0	2n+0	C^1+D^2	6	42	42
58	$(AuL)_2Fe(CO)_4$	6(3)	4n+0	2n+0	C^1+D^2	6	42	42
59	$(AuL)_3V(CO)_5$	9(4)	4n-2	2n+1	C^2+D^2	6	54	54
60	$(AuL)_3Re(CO)_4$	9(4)	4n-2	2n+1	C^2+D^2	6	54	54
61	$(AuL)_3Mn(CO)_4$	9(4)	4n-2	2n+1	C^2+D^2	6	54	54
62	$(AuL)_5Fe(CO)_3^{+1}$	15(6)	4n-6	2n+3	C^4+D^2	6	78	78
63	$(AuL)_6Mn(CO)_3^{+1}$	18(7)	4n-8	2n+4	C^5+D^2	6	90	90
64	$(AuL)_7Mo(CO)_3^{+1}$	21(8)	4n-10	2n+5	C^6+D^2	6	102	102
65	$(AuL)_7Mo(CO)_3^{+1}$	21(8)	4n-10	2n+5	C^6+D^2	6	102	102
66	$(AuL)_8Pt(CO)_2^{+}$	24(9)	4n-12	2n+6	C^7+D^2	6	114	114
67	$Pt(AuL)_8Au(CN)_2^{+}$	27(10)	4n-14	2n+7	C^8+D^2	6	126	126
68	$Pt(AuL)_8Au(CN)_2^{+}$	27(10)	4n-14	2n+7	C^8+D^2	6	126	126
69	$(AuL)_6(AuCl)_3Pt(CO)$	27(10)	4n-14	2n+7	C^8+D^2	6	126	126
70	$Pd(AuL)_{11}(AuCl)^{3+}$	36(13)	4n-20	2n+10	$C^{11}+D^2$	6	162	162
71	$Pd(AuL)_{11}(AuCl)^{3+}$	36(13)	4n-20	2n+10	$C^{11}+D^2$	6	162	162
72	$Pt_3Au_{10}L_{12}^{2+}$	36(13)	4n-20	2n+10	$C^{11}+D^2$	6	162	162
73	**$Os_{17}(CO)_{36}^{2-}$**	**38(17)**	**4n-28**	**2n+14**	**$C^{15}+D^2$**	**6**	**210**	**210**
74	**B_2H_6**	**2(2)**	**4n+4**	**2n-2**	**$C^{-1}+D^3$**	**8**	**12**	**12**
75	**$Re_2H_2(CO)_8$**	**2(2)**	**4n+4**	**2n-2**	**$C^{-1}+D^3$**	**8**	**32**	**32**
76	$Re_4H_4(CO)_{12}$	8(4)	4n+0	2n+0	C^1+D^3	8	56	56
77	$(AuL)_6W(CO)_4$	17(7)	4n-6	2n+3	C^4+D^3	8	92	92
78	$Pt(AuL)_6Au(CN)_2(CO)^{+}$	20(8)	4n-8	2n+4	C^5+D^3	8	104	104
79	$Au_{13}L_{12}^{3+}$	35(13)	4n-18	2n+9	$C^{10}+D^3$	8	164	164
80	$PtAu_{12}L_{12}^{2+}$	35(13)	4n-18	2n+9	$C^{10}+D^3$	8	164	164
81	$PtAu_{12}L_{12}^{2+}$	35(13)	4n-18	2n+9	$C^{10}+D^3$	8	164	164
82	$Au_{13}L_{12}^{3+}$	35(13)	4n-18	2n+9	$C^{10}+D^3$	8	164	164
83	**$Pd_{28}Au_4(CO)_{22}L_{12}$**	**92(32)**	**4n-48**	**2n+28**	**$C^{29}+D^3$**	**8**	**392**	**392**
84	B_3H_7	4(3)	4n+4	2n-2	$C^{-1}+D^4$	10	16	16
85	B_4H_6	7(4)	4n+2	2n-1	C^0+D^4	10	18	18
86	**$Re_3H_3(CO)_{10}^{2-}$**	**4(3)**	**4n+4**	**2n-2**	**$C^{-1}+D^4$**	**10**	**46**	**46**
87	$Re_4H_5(CO)_{12}^{-1}$	7(4)	4n+2	2n-1	C^0+D^4	10	58	58
88	$Os_3Cl(CO)_{10}(AuL)$	7(4)	4n+2	2n-1	C^0+D^4	10	58	58
89	$(AuL)_6AuCo_2(CO)_6^{+1}$	22(9)	4n-8	2n+4	C^5+D^4	10	118	118
90	$(AuL)_6AuCo_2(CO)_6^{+1}$	22(9)	4n-8	2n+4	C^5+D^4	10	118	118
91	$(AuL)_6AuCo_2(CO)_6^{+1}$	22(9)	4n-8	2n+4	C^5+D^4	10	118	118
92	**$Pd_{22}Au(CO)_{20}L_8^{+1}$**	**64(23)**	**4n-36**	**2n+18**	**$C^{19}+D^4$**	**10**	**286**	**286**
93	**$Os_3(CO)_{12}$**	**3(3)**	**4n+6**	**2n-3**	**$C^{-3}+D^5$**	**12**	**48**	**48**
94	$Re_3H_3(CO)_{12}$	3(3)	4n+6	2n-3	$C^{-2}+D^5$	12	48	48
95	B_3H_9	3(3)	4n+6	2n-3	$C^{-2}+D^5$	12	18	18
96	B_4H_8	6(4)	4n+4	2n-2	$C^{-1}+D^5$	12	20	20
97	$Os_4(CO)_{14}$	6(4)	4n+4	2n-2	$C^{-1}+D^5$	12	60	60
98	$Re_4H_4(CO)_{13}^2$	6(4)	4n+4	2n-2	$C^{-1}+D^5$	12	60	60

99	$Rh_4(CO)_{12}$	6(4)	4n+4	2n-2	$C^{-1}+D^5$	12	60	60
100	$(AuL)_3H_2ReL_3$	6(4)	4n+4	2n-2	$C^{-1}+D^5$	12	60	60
101	$(AuL)_3H_2ReL_3$	6(4)	4n+4	2n-2	$C^{-1}+D^5$	12	60	60
102	B_5H_7	9(5)	4n+2	2n-1	C^0+D^5	12	22	22
103	$FeCo_3(CO)_{12}(AuL)$	9(5)	4n+2	2n-1	C^0+D^5	12	72	72
104	$Os_5(CO)_{16}$	9(5)	4n+2	2n-1	C^0+D^5	12	72	72
105	$H_2Fe_4B(CO)_{12}^{-1}$	9(5)	4n+2	2n-1	C^0+D^5	12	72	72
106	$FeCo_3(CO)_{12}(AuL)$	9(5)	4n+2	2n-1	C^0+D^5	12	72	72
107	$H_2Fe_4B(CO)_{12}^{-1}$	9(5)	4n+2	2n-1	C^0+D^5	12	72	72
108	$FeCo_3(CO)_{12}(AuL)$	9(5)	4n+2	2n-1	C^0+D^5	12	72	72
109	$H_2Fe_4B(CO)_{12}^{-1}$	9(5)	4n+2	2n-1	C^0+D^5	12	72	72
110	$Os_4H_2(AuL)_2(CO)_{12}$	12(6)	4n+0	2n+0	C^1+D^5	12	84	84
111	$Re_4(CO)_{13}(AuL)_2$	12(6)	4n+0	2n+0	C^1+D^5	12	84	84
112	$Os_6(CO)_{18}$	12(6)	4n+0	2n+0	C^1+D^5	12	84	84
113	$Os_4H_2(AuL)_2(CO)_{12}$	12(6)	4n+0	2n+0	C^1+D^5	12	84	84
114	$Re_4(CO)_{13}(AuL)_2$	12(6)	4n+0	2n+0	C^1+D^5	12	84	84
115	$Os_4H_2(AuL)_2(CO)_{12}$	12(6)	4n+0	2n+0	C^1+D^5	12	84	84
116	$Re_4(CO)_{13}(AuL)_2$	12(6)	4n+0	2n+0	C^1+D^5	12	84	84
117	$CoRu_3(CO)_{12}(AuL)_3$	15(7)	4n-2	2n+1	C^2+D^5	12	96	96
118	$Ru_3(CO)_{12}(AuL)_3$	15(7)	4n-2	2n+1	C^2+D^5	12	96	96
119	$CoRu_3(CO)_{12}(AuL)_3$	15(7)	4n-2	2n+1	C^2+D^5	12	96	96
120	$Ru_3(CO)_{12}(AuL)_3$	15(7)	4n-2	2n+1	C^2+D^5	12	96	96
121	$Pd_9Tl(CO)_9L_6^{+1}$	24(10)	4n-8	2n+4	C^5+D^5	12	122	122
122	$Pd_9Tl(CO)_9L_6^{+1}$	24(10)	4n-8	2n+4	C^5+D^5	12	122	122
123	$Os_8(C)(CO)_{20}(AuL)_4$	30(12)	4n-12	2n+6	C^7+D^5	12	156	156
124	$Os_8(C)(CO)_{20}(AuL)_4$	30(12)	4n-12	2n+6	C^7+D^5	12	156	156
125	$Rh_{14}(CO)_{26}^{2-}$	36(14)	4n-16	2n+8	C^9+D^5	12	180	180
126	$Os_{10}(CO)_{24}(AuL)_4$	36(14)	4n-16	2n+8	C^9+D^5	12	180	180
127	$Rh_{15}(CO)_{27}^{3-}$	39(15)	4n-18	2n+9	$C^{10}+D^5$	12	192	192
128	$Rh_{17}(CO)_{30}^{3-}$	45(17)	4n-22	2n+11	$C^{12}+D^5$	12	216	216
129	**$Rh_{22}(CO)_{37}^{4-}$**	**60(22)**	**4n-32**	**2n+16**	**$C^{17}+D^5$**	**12**	**276**	**276**
130	$Re_4(CO)_{16}^{2}$	5(4)	4n+6	2n-3	$C^{-2}+D^6$	14	62	62
131	$Os_4(CO)_{15}$	5(4)	4n+6	2n-3	$C^{-2}+D^6$	14	62	62
132	B_4H_{10}	5(4)	4n+6	2n-3	$C^{-2}+D^6$	14	22	22
133	B_5H_9	8(5)	4n+4	2n-2	$C^{-1}+D^6$	14	24	24
134	$Re_5(C)(CO)_{16}(H)^{3-}$	8(5)	4n+4	2n-2	$C^{-1}+D^6$	14	74	74
135	$Os_5H_2(CO)_{16}$	8(5)	4n+4	2n-2	$C^{-1}+D^6$	14	74	74
136	B_6H_8	11(6)	4n+2	2n-1	C^0+D^6	14	26	26
137	$Os_6(CO)_{18}^{2-}$	11(6)	4n+2	2n-1	C^0+D^6	14	86	86
138	$Re_6(C)(CO)_{19}^{2-}$	11(6)	4n+2	2n-1	C^0+D^6	14	86	86
139	$Rh_6(CO)_{16}$	11(6)	4n+2	2n-1	C^0+D^6	14	86	86
140	$Rh_7(CO)_{16}^{3-}$	14(7)	4n+0	2n+0	C^1+D^6	14	98	98
141	$Os_7(CO)_{21}$	14(7)	4n+0	2n+0	C^1+D^6	14	98	98
142	$Re_7(C)(CO)_{21}^{3-}$	14(7)	4n+0	2n+0	C^1+D^6	14	98	98
143	$Re_8(C)(CO)_{24}^{2-}$	17(8)	4n-2	2n+1	C^2+D^6	14	110	110
144	$Os_8(CO)_{22}^{2-}$	17(8)	4n-2	2n+1	C^2+D^6	14	110	110
145	$Os_9(CO)_{24}^{2-}$	20(9)	4n-4	2n+2	C^3+D^6	14	122	122
146	$Rh_9(CO)_{19}^{3-}$	20(9)	4n-4	2n+2	C^3+D^6	14	122	122
147	$Os_{10}(CO)_{26}^{2-}$	23(10)	4n-6	2n+3	C^4+D^6	14	134	134
148	$Ni_6(C)(CO)_9(AuL)_4$	23(10)	4n-6	2n+3	C^4+D^6	14	134	134

149	$Os_8(CO)_{22}(AuL)_2$	23(10)	4n-6	2n+3	C^4+D^6	14	134	134
150	$Ni_6(C)(CO)_9(AuL)_4$	23(10)	4n-6	2n+3	C^4+D^6	14	134	134
151	$Os_8(CO)_{22}(AuL)_2$	23(10)	4n-6	2n+3	C^4+D^6	14	134	134
152	$Ni_6(C)(CO)_9(AuL)_4$	23(10)	4n-6	2n+3	C^4+D^6	14	134	134
153	$Os_8(CO)_{22}(AuL)_2$	23(10)	4n-6	2n+3	C^4+D^6	14	134	134
154	$Rh_{13}(CO)_{24}(H)^{4-}$	32(13)	4n-12	2n+6	C^7+D^6	14	170	170
155	$Pd_{28}Au_2(CO)_{26}L_{10}$	83(30)	4n-46	2n+23	$C^{24}+D^6$	14	374	374
156	$Pt_{38}(CO)_{44}^{2-}$	107(38)	4n-62	2n+31	$C^{32}+D^6$	14	470	470
157	**$HNi_{38}Pt_6(CO)_{48}^{5-}$**	**125(44)**	**4n-74**	**2n+37**	**$C^{38}+D^6$**	**14**	**542**	**542**
158	**$Re_4H_4(CO)_{15}^{2-}$**	**4(4)**	**4n+8**	**2n-4**	**$C^{-3}+D^7$**	**16**	**64**	**64**
159	$Rh_5(CO)_{15}^{-1}$	7(5)	4n+6	2n-3	$C^{-2}+D^7$	16	76	76
160	$Os_5(CO)_{18}$	7(5)	4n+6	2n-3	$C^{-2}+D^7$	16	76	76
161	B_5H_{11}	7(5)	4n+6	2n-3	$C^{-2}+D^7$	16	26	26
162	B_6H_{10}	10(6)	4n+4	2n-2	$C^{-1}+D^7$	16	28	28
163	$Os_6(CO)_{19}H_2$	10(6)	4n+4	2n-2	$C^{-1}+D^7$	16	88	88
164	B_7H_9	13(7)	4n+2	2n-1	C^0+D^7	16	30	30
165	$Rh_7(CO)_{15}(N)^{2-}$	13(7)	4n+2	2n-1	C^0+D^7	16	100	100
166	$Fe_4Au_4(CO)_{16}^{4-}$	16(8)	4n+0	2n+0	C^1+D^7	16	112	112
167	$Pd_{21}Au_2(CO)_{20}L_{10}$	61(23)	4n-30	2n+15	$C^{16}+D^7$	16	292	296
168	$Pd_{28}Au_4(CO)_{22}L_{16}$	88(32)	4n-48	2n+24	$C^{25}+D^7$	16	400	400
169	$Pd_{28}Au_8(CO)_{22}L_{16}$	88(32)	4n-48	2n+24	$C^{25}+D^7$	16	400	400
170	$Pd_{32}Au_4(CO)_{28}L_{14}$	100(36)	4n-56	2n+28	$C^{29}+D^7$	16	448	448
171	**$Fe_{14}Au_{34}(CO)_{50}^{6-}$**	**136(48)**	**4n-80**	**2n+40**	**$C^{41}+D^7$**	**16**	**592**	**592**
172	**$Os_5(CO)_{19}$**	**6(5)**	**4n+8**	**2n-4**	**$C^{-5}+D^8$**	**18**	**78**	**78**
173	B_6H_{12}	9(6)	4n+6	2n-3	$C^{-2}+D^8$	18	30	30
174	$Rh_6(CO)_{15}(N)^{-1}$	9(6)	4n+6	2n-3	$C^{-2}+D^8$	18	90	90
175	$Rh_6(CO)_{15}(C)^{2-}$	9(6)	4n+6	2n-3	$C^{-2}+D^8$	18	90	90
176	$Os_6(CO)_{17}L_4$	9(6)	4n+6	2n-3	$C^{-2}+D^8$	18	90	90
177	B_7H_{11}	12(7)	4n+4	2n-2	$C^{-1}+D^8$	18	32	32
178	$Os_7(CO)_{22}H_2$	12(7)	4n+4	2n-2	$C^{-1}+D^8$	18	102	102
179	**B_8H_{10}**	**15(8)**	**4n+2**	**2n-1**	**C^0+D^8**	**18**	**34**	**34**
180	**B_6H_{14}**	**8(6)**	**4n+8**	**2n-4**	**$C^{-3}+D^9$**	**20**	**32**	**32**
181	B_9H_{11}	17(9)	4n+2	2n-1	C^0+D^9	20	38	38
182	$B_{11}H_9$	23(11)	4n-2	2n+1	C^2+D^9	20	42	42
183	$Rh_{15}(CO)_{28}C_2^{-1}$	35(15)	4n-16	2n+5	C^6+D^9	20	200	200
184	**$Ni_{12}Au_6(CO)_{24}^{2-}$**	**44(18)**	**4n-16**	**2n+8**	**C^9+D^9**	**20**	**480**	**480**
185	**B_9H_{13}**	**16(9)**	**4n+4**	**2n-2**	**$C^{-1}+D^{10}$**	**22**	**40**	**40**
186	$Rh_9(CO)_{21}P^{2-}$	16(9)	4n+4	2n-2	$C^{-1}+D^{10}$	22	130	130
187	**$B_{10}H_{12}$**	**19(10)**	**4n+2**	**2n-1**	**C^0+D^{10}**	**22**	**42**	**42**
188	**$B_{11}H_{13}$**	**21(11)**	**4n+2**	**2n-1**	**C^0+D^{11}**	**24**	**46**	**46**
189	$B_{14}H_{10}$	30(14)	4n-4	2n+2	C^3+D^{11}	24	52	52
190	$Fe_{10}Au_{21}(CO)_{40}^{5-}$	81(31)	4n-38	2n+19	$C^{20}+D^{11}$	24	396	396
191	**$Ni_{32}Au_6(CO)_{44}^{6-}$**	**102(38)**	**4n-52**	**2n+26**	**$C^{27}+D^{11}$**	**24**	**480**	**480**
192	**$B_{10}H_{16}$**	**17(10)**	**4n+6**	**2n-3**	**$C^{-2}+D^{12}$**	**26**	**46**	**46**
193	$B_{13}H_{13}$	26(13)	4n+0	2n+0	C^1+D^{12}	26	52	52
194	$B_{14}H_{12}$	29(14)	4n-2	2n+1	C^2+D^{12}	26	54	54
195	$B_{12}H_{14}$	23(12)	4n+2	2n-1	C^0+D^{12}	26	50	50
196	$Ni_{12}Au(CO)_{24}^{3-}$	26(13)	4n+0	2n+0	C^1+D^{12}	26	182	182
197	**$Ni_{12}Au(CO)_{24}^{3-}$**	**26(13)**	**4n+0**	**2n+0**	**C^1+D^{12}**	**26**	**182**	**182**
198	**$Rh_{17}(CO)_{32}S_2^{-3}$**	**37(17)**	**4n-6**	**2n+3**	**C^4+D^{13}**	**28**	**232**	**232**

199	$Rh_{23}(CO)_{38}N_4^{-1}$	55(23)	4n-18	2n+9	$C^{10}+D^{13}$	28	304	304
200	$\mathbf{Fe_{14}Au_{28}(CO)_{52}^{8-}}$	**112(42)**	**4n-56**	**2n+28**	$\mathbf{C^{29}+D^{13}}$	**28**	**532**	**532**
201	$Fe_{12}Au_{22}(CO)_{48}^{6-}$	86(34)	4n-36	2n+18	$C^{19}+D^{15}$	32	440	440

Table 6B. Matryoshka Clusters

202	$Sc_{12}Sn_{21}^{108-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
203	$Ti_{12}Sn_{21}^{96-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
204	$V_{12}Sn_{21}^{84-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
205	$Cr_{12}As_{21}^{51-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
206	$Mn_{12}As_{21}^{39-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
207	$Ni_{12}As_{21}^{3-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
208	$Co_{12}As_{21}^{15-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
209	$Cu_{12}Sn_{21}^{12-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
210	$Zn_{12}Sn_{21}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
211	$Mg_{12}Sn_{21}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	108	108
212	$Cu_{12}Sb_{21}^{9+}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
213	$Zn_{12}Bi_{21}^{21+}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
214	$Hg_{12}Pb_{21}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
215	$Ca_{12}Si_{21}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	108	108
216	$Li_{12}Se_{21}^{30+}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	108	108
217	$Ni_{12}Te_{21}^{18+}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
218	$Fe_{12}Ge_{21}^{48-}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
219	$Hg_{12}Te_{21}^{42+}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
220	$Cd_{12}P_{21}^{21+}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228
221	$Co_{12}Te_{21}^{6+}$	78(33)	4n-24	2n+12	$C^{13}+D^{20}$	42	228	228

SOME CHARACTERISTICS OF CHEMICAL CAPPING SERIES

There are some notable characteristics of the capping chemical clusters which are arranged according to D^z series. Among others, these include the inherent Rudolph (Rudolph, 1976) sequence of **series (ΔK=3, Δn=1)**, the cluster valence electrons, CVE being **EVEN NUMBERS** except the comparatively few mono-skeletal elements with odd number electrons. If we observe carefully, also Wade-Mingos rules (Wade, 1976; Mingos, 1972) are well accommodated for a wide range of clusters. In the case, of the 4N series method with its skeletal numbers, all from mono-skeletal to multi-skeletal elements can readily be categorized except lanthanides and actinides as demonstrated in Tables 6A and 6B.

MATRYOSHKA AS A SPECIAL CASE OF DOUBLE CAPPING NATURE OF CLUSTERS

The matryoshka clusters belong to the special clusters series S=4n-24, K=2n+12, K= $C^{13}C$[M20], K* =$C^{13}+D^{20}$. This symbol predicts that 20 skeletal elements will be surrounded by 13 capping skeletal elements. In actual fact, what is observed is just the opposite (Huang, et al, 2014; Xiang, et al, 2015) and the C^{13} is found to be a centered **icosahedron. A sample matryoshka clusters both hypothetical and known ones which was published earlier is reproduced here comparative purposes in line with double capping concept of clusters (Kiremire, 2018c).**

CLUSTER VALENCE ELECTRONS AND CLUSTER NUMBER OCCURING AS EVEN NUMBERS

It has also been observed that in general cluster valence electrons are associated with even numbers and that the cluster number is usually a whole number. Thus, in a cluster the skeletal elements must combine in such a way that the resultant cluster number is a whole number. As is indicated in Table 1, the K value occurs in multiples of 0.5. Let us use boron as an illustration. Boron has a K value of 2.5 and since the cluster number K has to be whole number, that is why in F= B_nH_m, the fragment B_n when n=even, m must be even and when n=odd, m must have an odd value (Housecroft & Sharpe, 2005). Thus, the boranes have formulas such as B_2H_4, B_2H_6, B_3H_5, B_3H_7, B_3H_9, B_4H_6, B_4H_8, B_4H_{10}, B_5H_7, B_5H_9, B_5H_{11}, B_6H_8, B_6H_{10}, B_6H_{12}, B_6H_{14}, B_6H_{16}, B_7H_9, B_7H_{11}, B_7H_{13}, B_7H_{15}, B_8H_{10}, B_8H_{12}, B_8H_{14}, B_8H_{16}, B_9H_{11}, B_9H_{13}, B_9H_{15}, B_9H_{17}, $B_{10}H_{12}$, $B_{10}H_{14}$, $B_{10}H_{16}$, $B_{11}H_{13}$, $B_{11}H_{15}$, $B_{11}H_{17}$, $B_{12}H_{14}$, $B_{12}H_{16}$ and $B_{12}H_{18}$.

Skeletal numbers and their skeletal valences are so flexible in constructing isomeric graphical structures as illustrated in Figure 30.

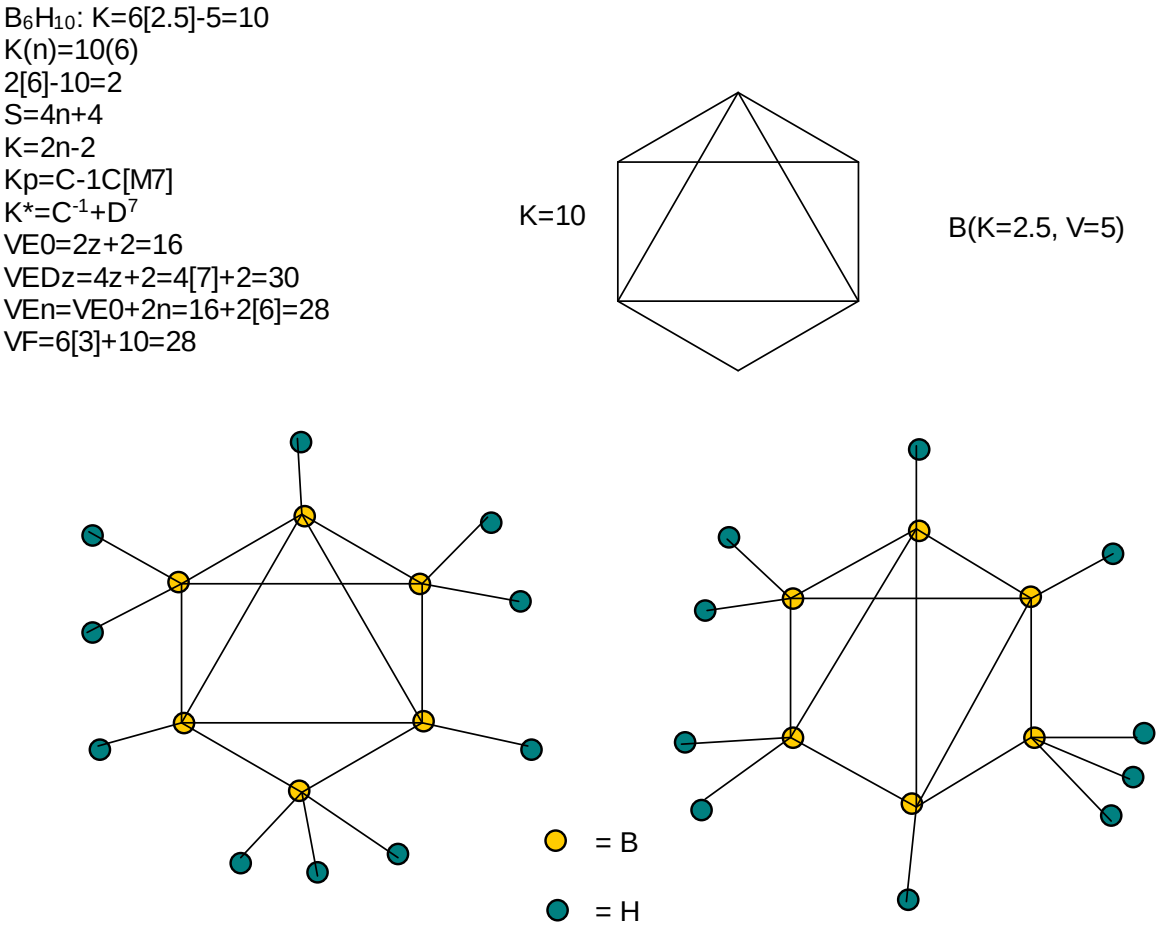


Figure 30. Isomeric graphical structures of structures of B_6H_{10}

4. Structural Prediction

The 4N series can act as a guide in structural prediction. The details of the geometrical shape can be ascertained by X-ray analysis. The categorization parameter $K^*=C^y+D^z$ recently developed can act as a guide for small values of y=0-12 and z=1-13. For example F= $Fe_6Pd_6H(CO)_{24}^{3-}$:K=6[5]+6[4]-0.5-24-1.5=28, K(n)=28(12), 2[12]-28=-4, S=4n-8, K=2n+4, $Kp=C^5C[M7]$, $K^*=C^5+D^7$, VE0=2z+2=2[7]+2=16,VE12=VE0+12n=16+12[12]=160, F=6[8]+6[10]+1+48+3=160. Since the capping theory gives us CVE=160 which is the same as obtained from the cluster formula, clearly vindicates its validity. According to the 4N series approach, the cluster is a penta-capped pentagonal bippyramid. Another similar example is $Ru_6Pd_6(CO)_{24}^{2-}$:K=6[5]+6[4]-24-1=29, K(n)=29(12), 2[12]-29=-5, S=4n-10, K=2n+5, $Kp=C^6C[M6]$, $K^*=C^6+D^6$, VE0=2z+2=14, VE12=VE0+12n=14+12[12]=158, VF=6[8]+6[10]+48+2=158. This example also shows that the capping model is correct. The cluster can be described as an octahedral fragment surrounded by six capping elements or the cluster is a hexa-capped octahedron. As for giant clusters with large nuclearity index, we can only describe them in terms of the nuclear size (z) and the number capping elements. A good example is $HNi_{38}Pt_6(CO)_{48}^{5-}$; $K^*=C^{38}+D^6$, which we can describe as a cluster with an octahedral shaped nucleus surrounded by 38 capping elements. This prediction is what is actually observed (Rossi & Zanello, 2011). What is interesting in this cluster is that all the octahedral fragment comprises of six platinum elements only. This type of predicting the shapes is what is reflected in Tables 5, 6A and 6B.

5. Conclusions

A wide range of clusters have been categorized using skeletal numbers. Categorization of each cluster has been expressed in the form $K^*=C^y+D^z$. It has been proposed that the symbol K* be referred to a categorization parameter. Clearly, arranging chemical clusters according to clan series (D^z) and family series (C^y) is easier and faster. The genesis electrons for any D^z clan tree are given by VE0 =2z+2. The six fundamental equations for calculating cluster valence electrons (CVE) have been

demonstrated. Despite the fact that only more than 200 clusters have been categorized, the method indicates that all elements of the periodic table and their clusters except lanthanides and actinides, can readily be arranged according to D^z and C^y series. This tremendously underpins the great insight of Rudolph of more than 40 years ago (Rudolph, 1976).

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