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Categorization and Structual Determination of Simple and More Complex Carbonyl Clusters of Rhenium and Osmium using K-values and the Cluster Table

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ABSTRACT

The shapes of conventional covalent compounds of main group elements and transition metal complexes can usually be deduced from their formulas. However, this is not the case for transition metal carbonyl clusters whose structures more or less resemble those of boranes and carboranes. Tremendous interest in the shapes of metal carbonyl clusters have been kept alive for more than five decades. Polyhedral skeletal theory, Jemmis rules, graph theory, and topological theory among others have been put forward so as to understand the structures of transition metal carbonyl clusters. This paper presents a highly simplified user friendly cluster table based on k-values which can be utilized together with an empirical formula to deduce the symmetries of simple to more complex cluster carbonyl complexes without any background of cluster theories. This approach highly complements the existing theories, in particular, the renowned polyhedral skeletal electron pair theory (PSEPT).

Key words: Carbonyl clusters, Rhenium, Osmium, K-values.

INTRODUCTION

Recently, a cluster table for transition metal carbonyls and has been designed to assist in the categorization of clusters and tentative assignment of geometries of clusters[1-5]. The cluster table has been re-arranged in such way that it has become much more user friendly. In this way, a given cluster can easily be categorized and its geometry tentatively assigned.

The cluster number, k-value for a carbonyl cluster is calculated[1-5] using the empirical formula $k = ½ (E-V)$. By analyzing the cluster numbers, it has been possible to discern the latent infinite world of series of clusters for elements which obey the 18-electron rule or 8-electron rule(octet rule). Some of these series have been organized and are presented in Table 1. In the newly reorganized and simplified table, the columns represent M_x values where x = 2,3, 4, 5, 6, and so on. In this new table,the

movement down an M_x column is like driving along a 'highway'. The movement crosses the columns ofdifferent cluster series that vary by "k = ± 1.That is, a change of one linkage or bond while the number of skeletal atoms remains the same. It is similar to adding or removing a monodentateligand (a pair of electrons) step by step. The horizontal movement along the series represents a progressive change in "k = ±2 and a change of M_x value by 1. The series comprises of different cluster values(k values) but belong to the same broad category type such as closo, nidoor arachno and so on. In a way each box or square in Table 1 may be regarded to be similar to a 'clan' which has many 'family' member series. Thus, the box can represent members from, rhenium, ruthenium or osmium 'families'or any other familyand so on. The diagonal movement represent a process in which there is a progressive change by "k = ± 3 and M_x by 1 as you shift from one type of 'cluster clan'series to another. This corresponds to a capping process.

RESULTS AND DISCUSSION

A selected range of carbonyl clusters taken mainly from rhenium element have been used as illustrations to categorize the clusters. Theresults re given inTable 2.In almost all cases categorization of clusters using the empirically calculated k-value and the cluster Table 1 are in agreement with those obtained by the known methods. A few examples are hereby given to illustrate the ease of utilizing the cluster table for categorizing a given cluster from its molecular formula.

1. $Re_4(H)_4(CO)_{13}^{2-}$; E = 4X18 = 72, V = 7x4 +4+ 13x2+2 = 60; k = ½ (E-V) = ½ (72-60) = 6. 'Raw code' of the cluster is represented as M-4-6-60:- where M refers to the cluster skeletal element, 4 –the number of skeletal elements, 6-the number of skeletal bonds or linkages, and 60 the total number of valence electrons. Table 1 has been constructed using a series of raw codes. In order to determine the type of cluster series it belongs to, we look at the cluster Table 1 under 'M-4 highway'. The M-4 highway is scanned until the raw code M-4-6-60 is found. Keeping on the same row, moving to the left, it is found that the raw code is in line with letter N(N = nido). Hence, the cluster is categorized as M-4-6-60-N. Therefore the cluster, $Re_4(H)_4(CO)_{13}^{2-}$ is a member of Nidoclan series of 4 skeletal elements with a total of 60 electrons.The 4 skeletal atoms with 6 linkages are normally found to form an 'ideal' tetrahedral (T_d) geometry Fig.1.The shape is drawn as a projection looking at it from above.

M-4-6 shape looking at it from above

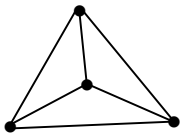
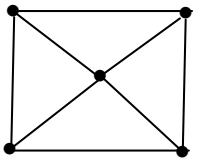


Fig. 1. Tetrahedral shape

2. $Re_5(C)(CO)_{16}(H)^{2-}$; E = 90, V = 74, k = ½ (E-V) = ½ (90-74) = 8. Raw code = M-5-8-74. As can be seen from Table 1, this cluster also belongs to the Nido family. The cluster category is M-5-8-74-N. The skeletal shape will be a square pyramidC_{4v}. This is shown in Fig. 2.

M-5-8 shape looking at it from above



Square pyramid

Fig, 2. M-5-8 shape

3. $Re_4(CO)_{16}^{2-}$; E = 72, V = 62, k = 5, raw code = M-4-5-62. Reading from M-4 highway column in table 1, the category code is M-4-5-62-A(arachno, butterfly shape). This shape is given in Fig. 3.

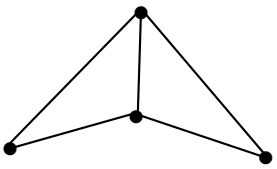
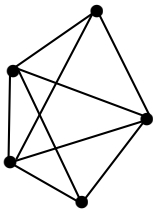


Fig. 3. The butterfly shape of M-4-5-62 cluster

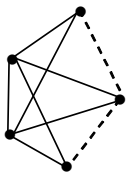
4. $Os_5(CO)_{16}$; The cluster has the derived category code of M-5-9-72-C. The complex belongs to the closo series. This is a geometry characteristic of regular trigonalbipyramid(D_{3h})shown in Fig. 4.



Trigonal bipyramid

Fig. 4. Shape of M-5-9 cluster

It is interesting to note[6] that the cluster complexex $RuIr_4(CO)_{15}^{2-}$(M-5-7-76-A), was found to have elongated trigonalbipyramid shape while on the other hand $Os_5(CO)_{16}$(M-5-9-72-C) was found to have regular trigonalbipyramid shape. The skeletal cluster shape of M-5-7 may be represented as indicated in Fig. 5.



Trigonal bipyramid elongated

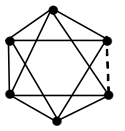
Fig. 5. Shape of M-5-7 cluster

It is not a surprise therefore that the two complexes (M-5-7-76-A) and (M-5-9-72-C) differ in length measurements as they truly belong to different series.

k-ISOMERISM

In some cluster systems with the same cluster code may exhibit different shapes which may be regarded as isomers. For instance[7], $Os_6(CO)_{18}^{2-}$(M-6-11-86-C) with k value of 11 has an octahedral shape, Fig. 6 while $O_6(H)_2(CO)_{18}$ (M-6-11-86-C) with k value of 11 has a mono-capped square pyramid, Fig. 7. Also the complexes[7] $Re_4(H)_4(CO)_{15}^{2-}$(E = 72, V = 64, k = ½ (E-V)= 4;from table cluster belongs to the Hypho series and code is M-4-4-64-H. Similarly, the cluster $Re_4(H)_4(CO)_{16}$ has a code M-4-4-64-H. However, the cluster shapes are different. The skeletal shapes are given in Fig. 8 and 9.

k = 11



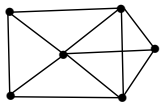
M-6-11-86-C,octahedral complex

Fig. 6.Shape of $Os_6(CO)_{18}^{2-}$

Looking at the square pyramid unit from top

k = 11

k = 8 + 3 = 11

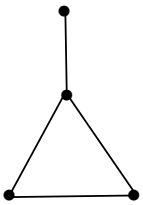


$Os_6(CO)_{18}(H)_2$

M-6-11-86-C

Fig. 7. Sketch of mono-capped square pyramid

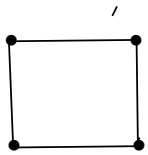
k = 4



M-4-4-64-H

Fig. 8. Skeletal shape of $Re_4(H)_4(CO)_{15}^{2-}$

k = 4



M-4-4-64-H

Fig. 9. Skeletal shape of $Re_4(H)_4(CO)_{16}$

More examples for illustration of the use of cluster table.

The osmium cluster $Os_6(CO)_{18}$ great interest[6]. It is considered as a bi-capped tetrahedron or mono-capped trigonalbipyramid. This observation is readily picked out from Table 1. The cluster category code of the complex is M-6-12-84-C^1C. As can be seen from the table, it is a mono-cap of M-5-9-72-C (trigonalbipyramid) which is diagonally below it and diagonally below M-5-9-72-C is M-4-4-6-60-N (a tetrahedralgeometry).This capping process is sketched in Fig. 10.

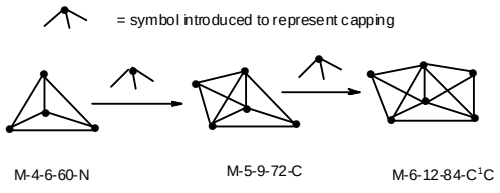


Fig. 10. The capping process from M-4-6-60-N to M-6-12-84-C^1C

Consider the complex $Au_3Ru_4(CO)_{12}L_3(H)$, L = PPh_3.

It is described as a tri-capped tetrahedron[6]. Its cluster series category code from the table is M-7-15-96-C^2C. Moving along the diagonal in the table, it is observed that it is a bi-cap of M-5-9-72-C(trigonalbipyramid). But M-5-9-72-C is a mono-cap of M-4-6-60-N(tetrahedral). Hence, in essence, it can be regarded as a tri-capped tetrahedron.

Let us take another example[8,9], $Os_6Pt_2(CO)_6(COD)_2$, COD= 4-electron donor. It has a cluster category code M-8-18-108-C^3C(M-5, difference between 8 and 3). From Table 1, it is a tri-cap based on trigonalbipyramid (M-5-9-72-C) as you move along M-8 diagonal. The skeletal shape of the cluster is is sketched as shown in Fig. 11.

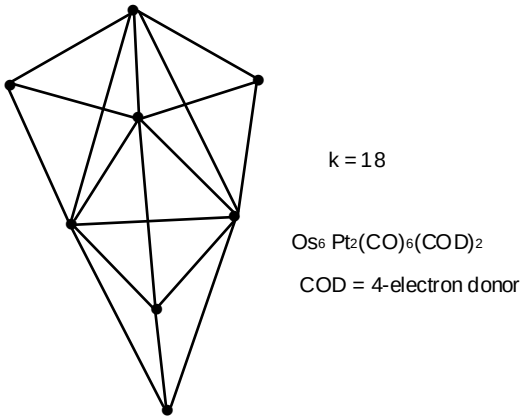


Fig. 11. Sketch of M-8-18-108-C^3C

The cluster k value can be considered to come from the M-5-9-72-C central unit contributing nine linkages and the three caps donating 3x3 =9 giving a rise of 9+ 9 = 18.

Let us look at another example[10], $Os_7(CO)_{19}Au_2(Ph_2CH_2PPh_2)$. In this case, E = 9x18=162, V=7x8+19x2+4 = 120. Hence, k = ½ (E-V) = ½ (162-120) =21. The corresponding cluster code for this complex will be M-9-21-120-C^4C(based on M-5 , specifically M-5-9-72-C as read from Table 1 diagonal). The sum of the linkages from this is 9 +4x3 =21 in agreement with the calculation. The skeletal sketch of the cluster is given in Fig.12.

The last example[11] we can use to illustrate the power of the empirical formula and cluster table is $Hg\{Fe_5(C)(CO)_{14}\}_2^{2-}$. For this complex, E = 11x18=198, V = 12+(5x8+4+14x2)x2+2 = 158,

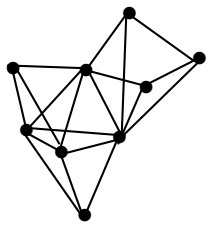


Fig. 12.The skeletal sketch of M-9-21-120-C^4C

k = ½ (E-V)= ½ (198-158) = 20. Hence, its code is M-11-20-158-N. Just by inspection of the k value and the formula, the k value can be split up as follows k =20 = 8+4+8. These can be regarded as linkage fragments which can tentatively give rise to the skeletal structure given in Fig. 13.

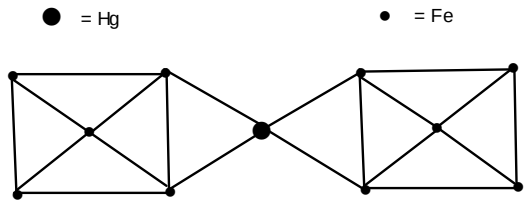


Fig. 13. Sketch of skeletal strucrure of M-11-20-158-N

The structure indicates two square pyramid units of Fe atoms drawn as seen from above linked to 4 bonds from Hg atom. The carbon atoms are not shown and stereochemistry not taken into account.

Identifying the beginning of the series from the k-value

There are two approaches in identifying the beginning of a series from a given k value. Consider the complex[7], $Os_9(H)(CO)_{24}^-$(M-9-20-122-C^3C). The complex has a k value of 20. The table shows that the cluster belongs to the clan members of M-9-20-122-C^3Cseries. Also the table shows that the three caps are bestowed onto an octahedral geometry(O_h). Furthermore from the code fragments M-9 and C^3, it can readily be deduced that the capping starts at M-6 which is specifically M-6-11-86-C in this case. The table also shows the

Table 1: Portion of Cluster Series of Transition Metal Carbonyls

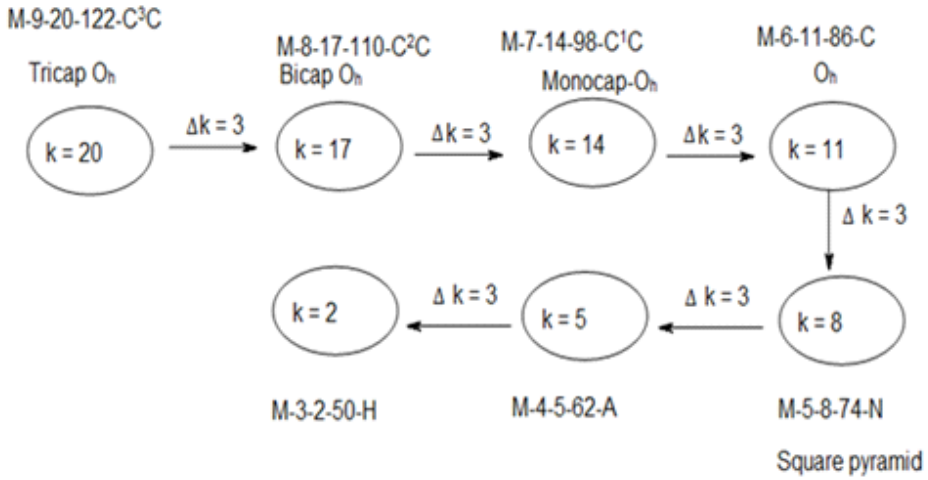
	M-2 10	M-3 12	M-4 14	M-5 16	M-6 18	M-7 20	M-8 22	M-9 24	M-10 26	M-11 28	M-12 30
C^7C	M-2-10-16 9	M-3-12-30 11	M-4-14-44 13	M-5-16-58 15	M-6-18-72 17	M-7-20-86 19	M-8-22-100 21	M-9-24-114 23	M-10-26-128 25	M-11-28-142 27	M-12-30-156 29
C^6C	M-2-9-18 8	M-3-11-32 10	M-4-13-46 12	M-5-15-60 14	M-6-17-74 16	M-7-19-88 18	M-8-21-102 20	M-9-23-116 22	M-10-25-130 24	M-11-27-144 26	M-12-29-158 28
C^5C	M-2-8-20 7	M-3-10-34 9	M-4-12-48 11	M-5-14-62 13	M-6-16-76 15	M-7-18-90 17	M-8-20-104 19	M-9-22-118 21	M-10-24-132 23	M-11-26-146 25	M-12-28-160 27
C^4C	M-2-7-22 6	M-3-9-36 8	M-4-11-50 10	M-5-13-64 12	M-6-15-78 14	M-7-17-92 16	M-8-19-106 18	M-9-21-120 20	M-10-23-134 22	M-11-25-148 24	M-12-27-162 26
C^3C	M-2-6-24 5	M-3-8-38 7	M-4-10-52 9	M-5-12-66 11	M-6-14-80 13	M-7-16-94 15	M-8-18-108 17	M-9-20-122 19	M-10-22-136 21	M-11-24-150 23	M-12-26-164 25
C^2C	M-2-5-26 4	M-3-7-40 6	M-4-9-54 8	M-5-11-68 10	M-6-13-82 12	M-7-15-96 14	M-8-17-110 16	M-9-19-124 18	M-10-21-138 20	M-11-23-152 22	M-12-25-166 24
C^1C	M-2-4-28 3	M-3-6-42 5	M-4-8-56 7	M-5-10-70 9	M-6-12-84 11	M-7-14-98 13	M-8-16-112 15	M-9-18-126 17	M-10-20-140 19	M-11-22-154 21	M-12-24-168 23
C	M-2-3-30 2	M-3-5-44 4	M-4-7-58 6	M-5-9-72 8	M-6-11-86 10	M-7-13-100 12	M-8-15-114 14	M-9-17-128 16	M-10-19-142 18	M-11-21-156 20	M-12-23-170 22
N	M-2-2-32 1	M-3-4-46 3	M-4-6-60 5	M-5-8-74 7	M-6-10-88 9	M-7-12-102 11	M-8-14-116 13	M-9-16-130 15	M-10-18-144 17	M-11-20-158 19	M-12-22-172 21
A	M-2-1-34 0	M-3-3-48 2	M-4-5-62 4	M-5-7-76 6	M-6-9-90 8	M-7-11-104 10	M-8-13-118 12	M-9-15-132 14	M-10-17-146 16	M-11-19-160 18	M-12-21-174 20
H	-1	M-3-2-50 1	M-4-4-64 3	M-5-6-78 5	M-6-8-92 7	M-7-10-106 9	M-8-12-120 11	M-9-14-134 13	M-10-16-148 14	M-11-18-162 16	M-12-20-176 18
H-1	-2	M-3-1-52 0	M-4-3-66 2	M-5-5-80 3	M-6-7-94 6	M-7-9-108 8	M-8-11-122 10	M-9-13-136 12	M-10-14-150 13	M-11-16-164 15	M-12-18-178 17
H-2			M-4-2-68	M-5-3-82	M-6-6-96	M-7-8-110	M-8-10-124	M-9-12-138	M-10-13-152	M-11-15-166	M-12-17-180

	M-11	M-12	M-13	M-14	M-15	M-16	M-17	M-18	M-19	M-20
	30	32	34	36	38	40	42	44	46	48
C^9C	M-11-30-138	M-12-32-152	M-13-34-166	M-14-36-180	M-15-38-194	M-16-40-208	M-17-42-222	M-18-44-236	M-19-46-250	M-20-48-264
	29	31	33	35	37	39	41	43	45	47
C^8C	M-11-29-140	M-12-31-154	M-13-33-168	M-14-35-182	M-15-37-196	M-16-39-210	M-17-41-224	M-18-43-238	M-19-45-252	M-20-47-266
	28	30	32	34	36	38	40	42	44	46
C^7C	M-11-28-142	M-12-30-156	M-13-32-170	M-14-34-184	M-15-36-198	M-16-38-212	M-17-40-226	M-18-42-240	M-19-44-254	M-20-46-268
	27	29	31	33	35	37	39	41	43	45
C^6C	M-11-27-144	M-12-29-158	M-13-31-172	M-14-33-186	M-15-35-200	M-16-37-214	M-17-39-228	M-18-41-242	M-19-43-256	M-20-45-270
	26	28	30	32	34	36	38	40	42	44
C^5C	M-11-26-146	M-12-28-160	M-13-30-174	M-14-32-188	M-15-34-202	M-16-36-216	M-17-38-230	M-18-40-244	M-19-42-258	M-20-44-272
	25	27	29	31	33	35	37	39	41	43
C^4C	M-11-25-148	M-12-27-162	M-13-29-176	M-14-31-190	M-15-33-204	M-16-35-218	M-17-37-232	M-18-39-246	M-19-41-260	M-20-43-274
	24	26	28	30	32	34	36	38	40	42
C^3C	M-11-24-150	M-12-26-164	M-13-28-178	M-14-30-192	M-15-32-206	M-16-34-220	M-17-36-234	M-18-38-248	M-19-40-262	M-20-42-276
	23	25	27	29	31	33	35	37	39	41
C^2C	M-11-23-152	M-12-25-166	M-13-27-180	M-14-29-194	M-15-31-208	M-16-33-222	M-17-35-236	M-18-37-250	M-19-39-264	M-20-41-278
	22	24	26	28	30	32	34	36	38	40
C^1C	M-11-22-154	M-12-24-168	M-13-26-182	M-14-28-196	M-15-30-210	M-16-32-224	M-17-34-238	M-18-36-252	M-19-38-266	M-20-40-280
	21	23	25	27	29	31	33	35	37	39
C	M-11-21-156	M-12-23-170	M-13-25-184	M-14-27-198	M-15-29-212	M-16-31-226	M-17-33-240	M-18-35-254	M-19-37-268	M-20-39-282
	20	22	24	26	28	30	32	34	36	38
N	M-11-20-158	M-12-22-172	M-13-24-186	M-14-26-200	M-15-28-214	M-16-30-228	M-17-32-242	M-18-34-256	M-19-36-270	M-20-38-284
	19	21	23	25	27	29	31	33	35	37
A	M-11-19-160	M-12-21-174	M-13-23-188	M-14-25-202	M-15-27-216	M-16-29-230	M-17-31-244	M-18-33-258	M-19-35-272	M-20-37-286
	18	20	22	24	26	28	30	32	34	36
H	M-11-18-162	M-12-20-176	M-13-22-190	M-14-24-204	M-15-26-218	M-16-28-232	M-17-30-246	M-18-32-260	M-19-34-274	M-20-36-288
	17	19	21	23	25	27	29	31	33	35
H-1	M-11-17-164	M-12-19-178	M-13-21-192	M-14-23-206	M-15-25-220	M-16-27-234	M-17-29-248	M-18-31-262	M-19-33-276	M-20-35-290
	16	18	20	22	24	26	28	30	32	34
H-2	M-11-16-166	M-12-18-180	M-13-20-194	M-14-22-208	M-15-24-222	M-16-26-238	M-17-28-250	M-18-30-264	M-19-32-278	M-20-34-292

Table 2: Categorization of Selected Carbonyl Cluster Complexes

Complex	E	V	k	Cluster Series * Category	Comment
$Re_2(H)_2(CO)_8$	36	32	2	M-2-2-32-N	Linear (double bond)
$Re_2(CO)_{10}$	36	34	1	M-2-1-34-A	Linear (single bond)
$Re_3(H)_3(CO)_{10}^{2-}$	54	46	4	M-3-4-46-N	Triangle
$Re_3(H)_2(CO)_{12}$	54	48	3	M-3-3-48-A	Triangle
$Re_4(H)_4(CO)_{15}^{2-}$	72	64	4	M-4-4-64-H	Square
$Re_4(H)_4(CO)_{13}^{2-}$	72	60	6	M-4-6-60-N	Tetrahedral (T_d)
$Re_4(H)_6(CO)_{12}^{2}$	72	60	6	M-4-6-60-N	Tetrahedral (T_d)
$Re_4(H)_5(CO)_{12}^{-}$	72	58	7	M-4-7-58-C	
$Re_4(CO)_{16}^{2-}$	72	62	5	M-4-5-62-A	Butterfly
$Re_4(H)_5(CO)_{14}$	72	62	5	M-4-5-62-A	Butterfly
$Re_4(H)_4(CO)_{12}$	72	56	8	M-4-8-56-C^1C	
$Re_5(C)(CO)_{16}(H)^{2-}$	90	74	8	M-5-8-74-N	Square pyramid (C_{4v})
$Re_6(H)_8(CO)_{18}^{2-}$	108	88	10	M-6-10-88-N	
$Re_6(C)(CO)_{19}^{2-}$	108	86	11	M-6-11-86-C	Octahedral (O_h)
$Re_6(C)(CO)_{19}(H)$	108	86	11	M-6-11-86-C	Octahedral (O_h)
$Re_6(C)(CO)_{18}(H)_2^{2}$	108	86	11	M-6-11-86-C	Octahedral (O_h)
$Re_6(C)(CO)_{18}(H)^{3}$	108	86	11	M-6-11-86-C	Octahedral (O_h)
$Re_7(C)(CO)_{21}^{3}$	126	98	14	M-7-14-98-C^1C	Monocap based on O_h(11+3 = 14)
$Re_7(C)(CO)_{21}(H)^{2}$	126	98	14	M-7-14-98-C^1C	Monocap based on O_h(11+3 = 14)
$Re_7(C)(CO)_{21}(H)_2$	126	98	14	M-7-14-98-C^1C	Monocap based on O_h(11+3 = 14)
$Re_7(C)(CO)_{22}$	126	98	14	M-7-14-98-C^1C	Monocap based on O_h(11+3 = 14)
$Re_8(C)(CO)_{22}$	144	110	17	M-8-17-110-C^2C	Bicap based on O_h(11+3+3 = 17)
$Os_5(CO)_{16}$	90	72	9	M-5-9-72-C	Trigonalbipyramid (TBP,D_{3h})
$Os_5(CO)_{15}(H)$	90	72	9	M-5-9-72-C	Trigonalbipyramid (TBP,D_{3h})
$Os_6(CO)_{18}$	108	84	12	M-6-12-84-C^1C	Monocap based on TBP(9+3 = 12)
$Os_6(CO)_{18}^{2}$	108	86	11	M-6-11-86-C	Octahedral (O_h)
$(H)Os_6(CO)_{18}$	108	86	11	M-6-11-86-C	Octahedral (O_h)
$(H)_2Os_6(CO)_{18}$	108	86	11	M-6-11-86-C	Square pyramid –monocap(8+3 = 11)
$Os_6(CO)_{17}L_4$ L = $P(OMe)_3$	108	90	9	M-6-9-90-A	A triangle on top of 2 atom linked triangles
$H)_2Os_6(CO)_{19}$	108	88	10	M-6-10-88-N	
$Os_7(CO)_{21}$	126	98	14	M-7-14-98-C^1C	Monocap based on O_h(11+3 = 14)
$Os_7(CO)_{21}(H)_2$	126	100	13	M-7-13-C	
$Os_7(CO)_{22}(H)_2$	126	102	12	M-7-12-N	
$(H)_2Os_7(CO)_{20}$ =14)	126	98	14	M-7-14-98-C^1C	Bicap T_d with a leg linkage(6+3+3+2
$Os_8(CO)_{22}^{2-}$	144	110	17	M-8-17-110-C^2C	Bicap based on O_h(11+3+3 =17)
$(H)Os_8(CO)_{22}^{2-}$	144	110	17	M-8-17-110-C^2C	2 Edge-fused T_d units each monocapped.
$Os_9(CO)_{24}^{2-}$	162	122	20	M-9-20-122-C^3C	Tricapped based on O_h(11+3+3+3) =20)
$Os_9(H)(CO)_{24}^{-}$	162	122	20	M-9-20-122-C^3C	Tricapped based on O_h(11+3+3+3) =20)
$Os_{10}(C)(CO)_{24}^{2-}$	180	134	23	M-10-23-134-C^4C	Tetracapped based on O_h(11+3+3+3+3 = 23)
$Os_{10}(CO)_{26}^{2-}$	180	134	23	M-10-23-134-C^4C	Tetracapped based on O_h(11+3+3+3+3 = 23)

*C = Closo, N = Nido, A = Arachno, H = Hypho, C^1c = Monocap, C^2c = Bicap, Etc, H-1 = First Series Below Hypho, H-2 = Second Series Below Hypho, Etc



Scheme 1: Shows the diagonal descent of k=20 to the

Table 3: e 3: Important cluster series normally encountered

M_x	k	V	Category Code	Corresponding Element Code Main Group	Possible skeletal geometry
2	1	34	M-2-1-34-A	M-2-1-14-A	Linear, single bond
2	2	32	M-2-2-32-N	M-2-2-12-N	Linear, double bond
2	3	30	M-2-3-30-C	M-2-3-10-C	Linear, Triple bond
2	4	28	M-2-4-28-C^1C	M-2-4-08-C^1C	Linear, Quadruple bond
3	3	48	M-3-3-48-A	M-3-3-18-A	Triangle
4	6	60	M-4-4-60-N	M-4-4-20-N	T_d
5	9	72	M-5-9-72-C	M-5-9-22-C	Trigonalbipyramid
5	8	74	M-5-8-74-N	M-5-8-24-N	Square pyramid
6	11	86	M-6-11-86-C	M-6-11-26-C	O_h
6	10	90	M-6-9-90-A	M-6-9-30-A	Trigonal Prism
7	14	98	M-7-14-98-C^1C	M-7-14-28-C^1C	Monocap-O_h
8	17	110	M-8-17-110-C^2C	M-8-17-300-C^2C	Bicap-O_h
9	20	122	M-9-20-122-C^3C	M-9-20-32-C^3C	Tricap-O_h
10	23	134	M-10-23-134-C^4C	M-10-23-34-C^4C	Tetracap-O_h

beginning cluster clan code can easily be traced. This will entail the de-capping descent of "k =3. This process is illustrated in scheme 1.

This scheme implies that beginning with a hypho cluster of 3 atoms with 2 linkages and 50 valence electrons we can successively generate a butterfly geometry (M-4-5-62-A), followed by a square pyramid geometry (M-5-8-74-N), octahedral geometry (M-6-11-86-C), until we arrive at a tri-capped octahedral geometry of (M-9-20-122-C^3C) cluster. The closo series begins with the code M-2-3-30 for two skeletal elements up to M-12-23-170 in the table. The series could be extended as far as possible. Although Table 1 is meant for transition metal carbonyl clusters, it can readily be adapted for use for main group element clusters.

Special cluster series

There are special cluster series that are usually encountered in chemistry. Some of these are given in Table 3.

Table 4: Magic Cluster Ratio

Code: M-x-k-V	Magic cluster ratio:-M-x:k:V
M-2-4-28	1:2:14
M-3-6-42	1:2:14
M-4-8-56	1:2:14
M-5-10-70	1:2:14
M-6-12-84	1:2:14
M-7-14-98	1:2:14
M-8-16-112	1:2:14
M-9-18-126	1:2:14
M-10-20-140	1:2:14
M-11-22-154	1:2:14
M-12-24-168	1:2:14
M-13-26-182	1:2:14
M-14-28-196	1:2:14
M-15-30-210	1:2:14
M-16-32-224	1:2:14
M-17-34-238	1:2:14
M-18-36-252	1:2:14
M-19-38-266	1:2:14
M-20-40-280	1:2:14

Magic cluster ratio (1:2:14)

Consider the cluster category code of the mono-cap series (C^1C). The selected ones are given in Table 4.

CONCLUSION

Simple and relatively more complex transition metal carbonyl clusters can be analyzed using basic number theory. The cluster number k value is obtained from the empirical formula k = ½ (E-V). The cluster numbers have been utilized to construct a user friendly cluster table for classifying clusters into category series. The cluster number, k value can be used to categorize a given carbonyl cluster. The k value may simply be regarded as the number of bonds or linkages or 'pillars' that hold a given cluster system together. Furthermore, from the k value with or without the help of the cluster table the skeletal geometry of the cluster may tentatively derived. By this approach, the skeletal structures of metal carbonyls from simple to relatively more complex can greatly be appreciated without prior knowledge of the polyhedral skeletal electron pair theory[12], Jemmis rules[13] or topology concepts[14]. Nevertheless, this work complements the existing knowledge on carbonyl clusters. Theauthor believes method will be enjoyed by a wide spectrum of scholars mainly undergraduate, postgraduate chemistry students as well as chemistry teachersin secondary schoolsor high schools due to its simplicity.

Dedication

This paper is dedicated to Charles Alfred Coulson(1910-1974) who once briefly taught the author in Africa, Gilbert Newton Lewis(1875-1946) and Irving Langmuir(1881-1957).

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