

Categorization of Boranes Into Clan Series

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Abstract

Boranes, despite their instability in nature, can be regarded as hydrocarbon relatives since a [BH] fragment corresponds to a carbon [C] skeletal element in terms of the number of valence electrons. The borane formula which can be expressed as B_nH_m usually appears in such a way that when (n) is even, then (m) is even and when (n) is odd, (m) is odd as well. Through the study of cluster series, it appears that the cluster number K which represents skeletal linkages is usually a whole number. This inherent characteristic confers unique order within borane clusters with nodal connectivity of 5 and the polyhedral nature of the borane clusters. The orderliness of the borane clusters is reflected by the ease of their categorization into clan series and their readily constructed geometrical isomeric structures. The cluster valence electrons can easily be calculated using one of the six recently discovered fundamental equations.

Keywords: isomeric structures, polyhedral triangles, valence equations, clusters, boranes, skeletal nodes

1. Introduction

Borane hydride clusters have fascinated and intrigued scientists since their discovery in 1912 due to their unique characteristic features of polyhedral shapes, apparent strange stoichiometries and bonding (Stock, 1933; Lipscomb, 1963; Wade, 1971, 1976; Jemmis, et al, 2001a-b; Mingos, 1984, Kiremire, 2014). Furthermore, some applications of borane clusters have been discovered and the field is expanding (Hawthorne, et al, 1990). Arising from their polyhedral shapes, certain names such as closo, nido, arachno, hypho and klapo (Housecroft and Sharpe, 2005; Meissler, et al, 2014) were associated with characteristic shapes. In addition, attempts to explain their structures have given rise to concepts such as Wade-Mingos rules (Mingos, 1972; Welch, 2013), Jemmis mno rules (Jemmis, et al, 2001b), styx numbers (Lipscomb, 1963), and topological theories (Teo, et al, 1984), among others. Closer analysis of clusters revealed that the skeletal elements and clusters from the main group and transition elements can be analyzed and categorized more extensively using the 4N series method and that they strictly obey the law of skeletal numbers and their valences (Kiremire, 2017a-b). In this paper, selected sample of boranes will be categorized according to their CLAN SERIES, D^z where D^z originates from the categorization cluster parameter $K^* = C^y + D^z$ (Kiremire, 2019a-c), the $K(n)$ parameter will be utilized to construct the polyhedral isomers of borane clusters and derive their cluster formulas and valence electrons. The skeletal numbers of elements and ligands discovered and utilized earlier are provided in appendix 1 and 2 for ease of reference and recognition as the concept is still new (Kiremire, 2017a).

2. Results and Discussion

2.1 The Skeletal Numbers and Skeletal Linkages

The skeletal elements of the periodic table particularly the main group and transition metals do possess intrinsic skeletal numbers (K) (Kiremire, 2016). These simply indicate the number of electron pairs a given skeletal element needs for it to achieve the 8-electron configuration (octet rule) for main group elements or the 18-electron configuration in the case of transition elements (2017c). When the skeletal number is doubled, then we get the number of skeletal linkages that can be attached to the element or the number of single electron donation the element requires to attain the respective 8 or 18 electron-rule. In the case of boron, $K=2.5$ which means it requires 2.5 electron pairs ($V=2 \times 2.5=5e$) so as to achieve the octet rule $=3+5=8$. Thus, since the boron atom has 3 electrons, when it receives 5 others, it achieves the noble gas configuration of 8. In principle, the boron skeletal element can be regarded as portraying 5 skeletal linkages in its cluster compounds. The skeletal numbers of other elements can be found in published articles (Kiremire 2019a-c).

2.2 Skeletal Elements as Nodes and Boron Exerting a Skeletal Valence of Five

In the case of boranes, we can regard the boron skeletal element as a node which can have 5 linkages around it since it has a skeletal number $K=2.5$ and $V=2K=5$). We know that a hydrogen element carries one electron and hence it is regarded as a single electron donor or ligand. In principle, we expect a boron skeletal element to form a simple mono-skeletal cluster with the formula BH_5 . But what is normally encountered is the cluster BH_4^- . According to the 4N series approach, (-1) charge is equivalent to a single H element. Therefore, we can consider BH_4^- as being derived from BH_5 by replacing (H) with (-1) charge. If the replacement process is continued, we end up with the ion B^{5-} . The possible species that can be generated are shown in Figure 1. According to the 4N series approach all the generated species are equivalent. That is, $BH_5 \equiv BH_4^- \equiv BH_3^{2-} \equiv BH_2^{3-} \equiv BH^+ \equiv B^{5-}$. When the cluster has two or more boron skeletal elements or NODES, each of the nodes will exert 5 linkages. This is shown in Figures 2 for B_2H_8 and its isomers and 3 for B_2H_6 and its bridged isomer. The $B_2H_7^-$ was identified and an IR studies conducted (Matsui & Taylor, 1989). The diborane molecule B_2H_6 is well known and has two bridging H ligands. The bridging structure can be viewed as a rearrangement of the 5-coordinated skeletal nodes. More than 60 isomeric graphical structures have been sketched according to the skeletal valence ($V=5$ =five skeletal or nodal linkages) of boron. Clearly, the concept of skeletal number and valence make a lot of sense in rationalizing the cluster formulas of many complexes.

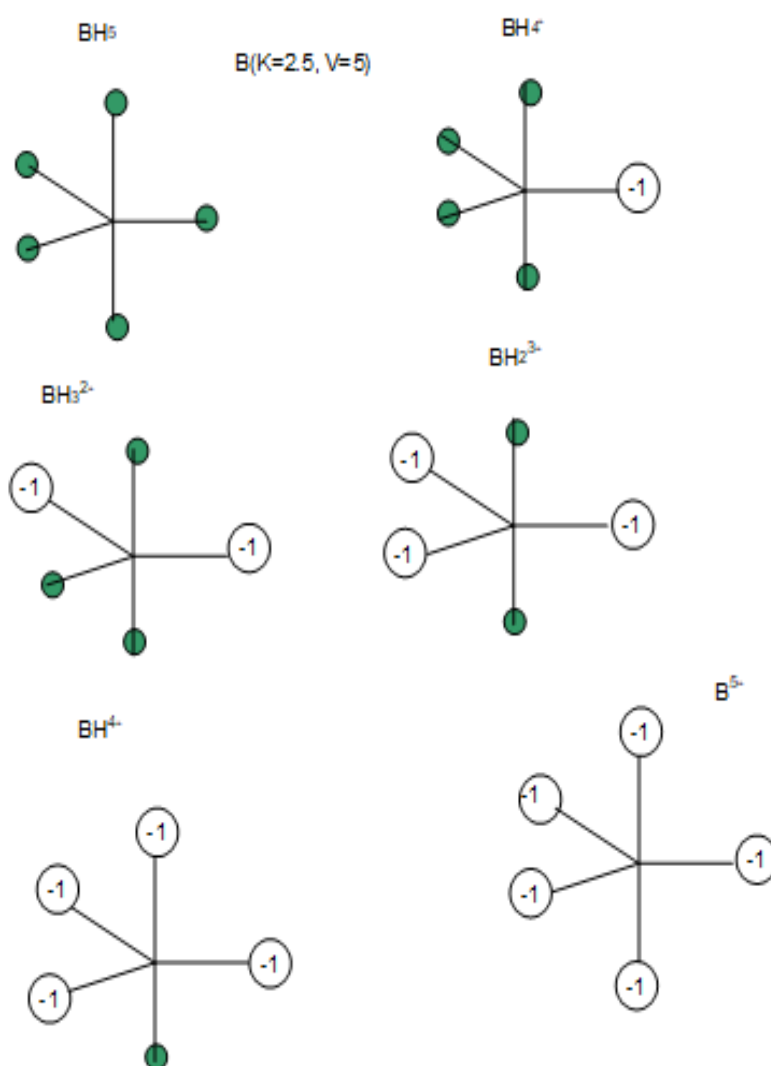


Figure 1. Equivalent isomeric structures of boron skeletal element

EX-1. B_2H_8
 $K=2[2.5]-8[0.5]=1, n=2$
 $K(n)=1(2)$
 $2[2]-1=3$
 $S=4n+6$
 $K=2n-3$
 $Kp=C^{-2}C[M4]$
 $K^*=C^{-2}+D^4$
 $y=-2, z=4$
 $VE_0=2z+2=2[4]+2=10$
 $VE=VE_0+2n=10+2[2]=14$
 $VF=2[3]+8=14$
 $VEDz=4z+2=4[4]+2=18$
 $VE=VEDz+2y=18+2[-2]=14$
 $VE=2y+4z+2=2[-2]+4[4]+2=14$
 $VE=8n-2K=8[2]-2[1]=14$
 $VE=4n+6=4[2]+6=14$
 $VE=VE_0+2y+2z=10+2[-2]+2[4]=14$

B_2H_8 : $K=1$, the 2 boron skeletal elements are linked by one bond.

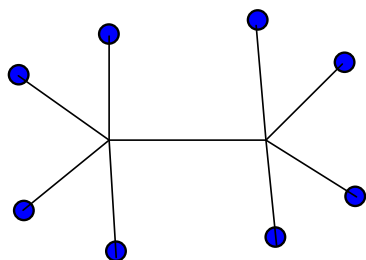


Figure 2A. Isomeric graphical structure of B_2H_8

$B(K=2.5, V=2K=5)$; Boron skeletal element has 5 skeletal linkages)

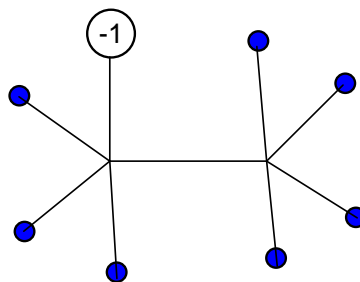


Figure 2B. Isomeric graphical structure of $B_2H_7^-$

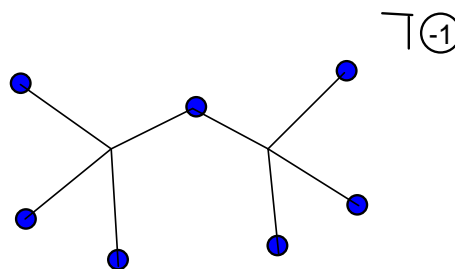


Figure 2C. Rearrangement of 2B

Boron skeletal element strictly conforms to a skeletal valence of 5

$$\begin{aligned}
 \text{EX-2. } B_2H_6: K &= 2[2.5] - 6[0.5] = 2, n = 2 \\
 K(n) &= 2(2) \\
 2[2] - 2 &= 2 \\
 S &= 4n + 4 \\
 VE &= 4[2] + 4 = 12 \\
 VF &= 2[3] + 6 = 12
 \end{aligned}$$

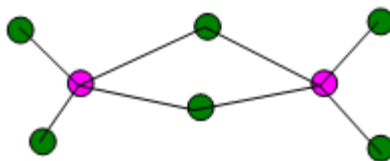
Figure 3. Isomeric graphical structure of B_2H_6 

Figure 4. Rarrangement of Figure 3

2.3 The Six Equations for Calculating the Cluster Valence Electrons

Some or all the six equations have been used in the analysis of many clusters (Kiremire, 2019b) are being applied here in the analysis of the selected borane clusters. They all give the same result of the cluster valence electrons (VE) as the one calculated from the cluster formula (VF). This underpins the validity of the developed cluster valence equations. They are derived from the series equations and the capping principle of the 4N series method. These equations are:

- i. $K(n)$; $VE = 8n - 2K$
- ii. $S = 4n + q$; $VE = 4n + q$
 $K = C^y + D^z$; $VE_0 = 2z + 2$, $VED_z = 4z + 2$, $y + z = n =$ the number of skeletal elements.
- iii. $VE = VE_0 + 2n$
- iv. $VE = VED_z + 2y$
- v. $VE = 2y + 4z + 2$
- vi. $VE = VE_0 + 2y + 2z$

The symbol $n =$ the number of skeletal elements in a cluster excluding the ligands, $K =$ skeletal linkages linking up the skeletal elements, $S =$ series equation, q is a numerical variable that defines the type of the cluster, the K value can also be expressed in terms of $C^y + D^z$ where C and D represent the categorization of a cluster, y is in principle, the number of the capping skeletal elements, and z is the number of the nuclear elements.

Some of these or all the equations will be applied in the analysis of the following cluster examples.

$$\begin{aligned}
 1. \text{ B}_3\text{H}_9: K &= 3[2.5] - 9[0.5] = 3, n = 3 \\
 K(n) &= 3(3) \\
 2[3] - 3 &= 3 \\
 S &= 4n + 6 \\
 K &= 2n - 3 \\
 K_p &= C^{-2}C[M5] \\
 K^* &= C^{-2} + D^5 \\
 y &= -2, z = 5 \\
 VE_0 &= 2z + 2 = 2[5] + 2 = 12 \\
 VE &= VE_0 + 2n = 12 + 2[3] = 18 \\
 VED_z &= 4z + 2 = 4[5] + 2 = 22 \\
 VE &= VED_z + 2y = 22 + 2[-2] = 18 \\
 VE &= 2y + 4z + 2 = 2[-2] + 4[5] + 2 = 18 \\
 VE &= VE_0 + 2y + 2z = 12 + 2[-2] + 2[5] = 18 \\
 VF &= 3[3] + 9 = 18 \\
 VE &= 8n - 2K = 8[3] - 2[3] = 18 \\
 VE &= 4n + 6 = 4[3] + 6 = 18
 \end{aligned}$$

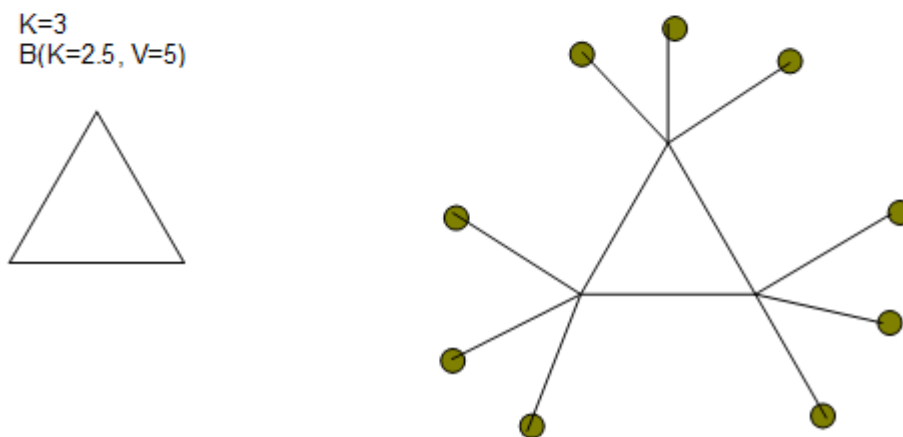


Figure 5. Isomeric graphical structure of B_3H_9

The cluster categorization is derived from the cluster series equation. The series equation is readily obtained from the following relationships.

$$S = 4n + q = VE \quad (\text{i})$$

$$VE = 8n - 2K \quad (\text{ii})$$

Another relationship is readily derived from these two equations as follows:

$$4n + q = 8n - 2K \quad (\text{iii})$$

$$q = 4n - 2K \quad (\text{iv})$$

$$q/2 = 2n - K \quad (\text{v})$$

Knowing the values of n and K of a cluster, the q value of a cluster can be derived from (V). Hence the cluster series equation can readily be obtained. From the series equation, the K value is then expressed in terms of n and q . The K_p value and K^* can also be derived from K . The K^* is finally expressed in terms of C^y and D^z which determine the categorization of a cluster. This approach has been applied in the example 1 given above.

$$\begin{aligned}
 2. F=B_4H_{10}:K=4[2.5]-5=5,n=4 \\
 K(n)=5(4) \\
 2[4]-5=3 \\
 S=4n+6 \\
 K=2n-3 \\
 Kp=C^{-2}C[M6] \\
 K^*=C^{-2}+D^6 \\
 y=-2, z=6 \\
 VE_0=2z+2=2[6]+2=14 \\
 VE=VE_0+2n=14+2[4]=14+8=22 \\
 VE=2y+4z+2=2[-2]+4[6]+2=22 \\
 VF=4[3]+10=22
 \end{aligned}$$

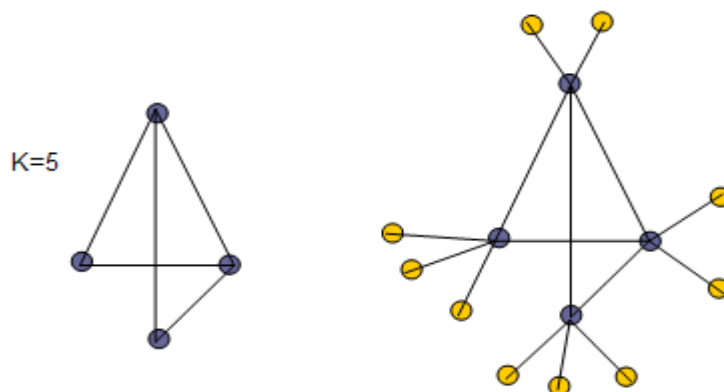


Figure 6. Isomeric graphical structure of B_4H_{10}

$$\begin{aligned}
 3. F=B_9H_{13}:K=9[2.5]-13[0.5]=16,n=9 \\
 K(n)=16(9) \\
 2[9]-16=2 \\
 S=4n+4 \\
 K=2n-2 \\
 Kp=C^{-1}C[M10] \\
 K^*=C^{-1}+D^{10} \\
 y=-1,z=10 \\
 VE_0=2z+2=2[10]+2=22 \\
 VE=VE_0+2n=22+2[9]=40 \\
 VE=VE_0+2y+2z=22+2[-1]+2[10]=40 \\
 VE=2y+4z+2=2[-1]+4[10]+2=40 \\
 VF=9[3]+13=40 \\
 VE=8n-2K=8[9]-2[16]=40 \\
 VE=4n+4=4[9]+4=40 \\
 VEDz=4z+2=4[10]+2=42 \\
 VE=VEDz+2y=42+2[-1]=40
 \end{aligned}$$

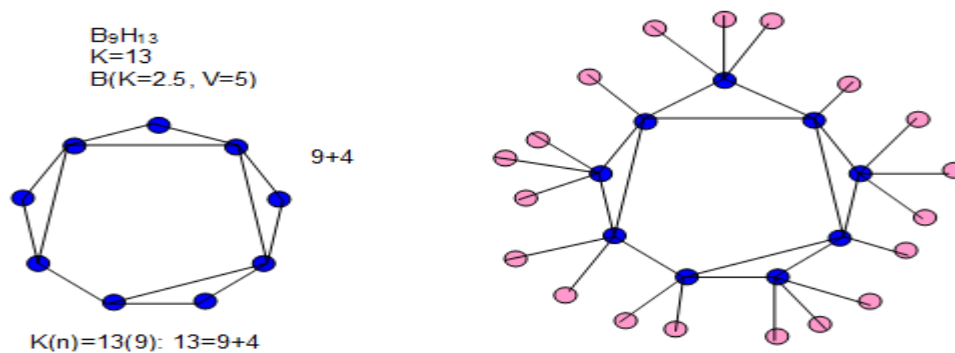


Figure 7. Isomeric graphical structure of B_9H_{13}

$$\begin{aligned}
 4. \quad F &= B_{14}H_{20}; K=14[2.5]-20[0.5]=25, n=14 \\
 K(n) &= 25(14) \\
 2[14]-25 &= 3 \\
 S &= 4n+6 \\
 K &= 2n-3 \\
 K_p &= C^{-2}C[M16] \\
 K^* &= C^{-2}+D^{18} \\
 y &= -2, z=16 \\
 VE &= 2z+2=2[16]+2=34 \\
 VE &= VE_0+2n=34+2[14]=62 \\
 VF &= 14[3]+20=62 \\
 VE &= VE_0+2y+2z=34+2[-2]+2[16]=62 \\
 VE &= 2y+4z+2=2[-2]+4[16]+2=62 \\
 VEDz &= 4z+2=4[16]+2=66 \\
 VE &= VEDz+2y=66+2[-2]=62 \\
 VE &= 8n-2K=8[14]-2[25]=62 \\
 VE &= 4n+6=4[14]+6=62
 \end{aligned}$$

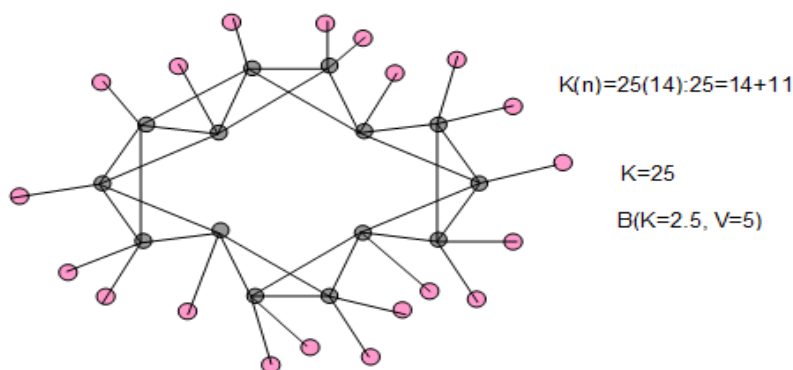


Figure 8. Isomeric graphical structure of $B_{14}H_{20}$

2.4 Construction of the Skeletal Isomeric Structures

Arising from the experience of sketching isomeric skeletal isomers of clusters, it has been found to be easier and useful to use quasi-circular skeletal structures to construct the isomers. The $K(n)$ parameter has been very helpful. In this regard, a geometrical figure of n sides is selected and K linkages are inserted. Let us consider the following examples as illustrations. Take $C_2B_4H_6$ cluster. The K value for C is 2 and $V=4$ whereas B has a K value of 2.5 and $V=5$. The cluster has 11 skeletal linkages and 6 skeletal elements. In order to construct a skeletal isomer, a 6-membered ring is selected. Then 5 linkages are added in such a way that TRIANGULAR FACES ARE FORMED. Since there are 6 skeletal elements, these can cyclically be linked by 6 linkages out of the 11 total linkages corresponding to $K=11$. Hence, the remaining 5 linkages are utilized to construct the appropriate triangular faces. The triangles are constructed in such a way that the valences of the constituent skeletal elements are obeyed. This is shown in Figure 9. The same approach was done for B_8H_{14} , $B_{10}H_{14}$, $C_2B_{10}H_{12}$ and B_{12} which are shown in Figures 10-17. The boron skeletal element is quite unique in that in it appears to strictly exert a skeletal valence of 5 in all its hydride clusters and other complexes such as halides, metalloboranes and metallocarboranes (Kiremire, 2017b). According to the $4N$ series approach, we can regard the bridging hydride structures of boranes as re-arrangements of the clusters so as to achieve more stable conformations. In summary, the construction of the isomeric shapes using the $K(n)$ parameter, can be expressed as $K=n+x$ where K =number of skeletal linkages, n = the number of the skeletal elements and x = the number of linkages inserted within and/or around the n -sided figure in such a way that skeletal TRIANGLES are generated. The parent structures on which linkage lines are drawn are based on Symyx Draw 3.2 program.

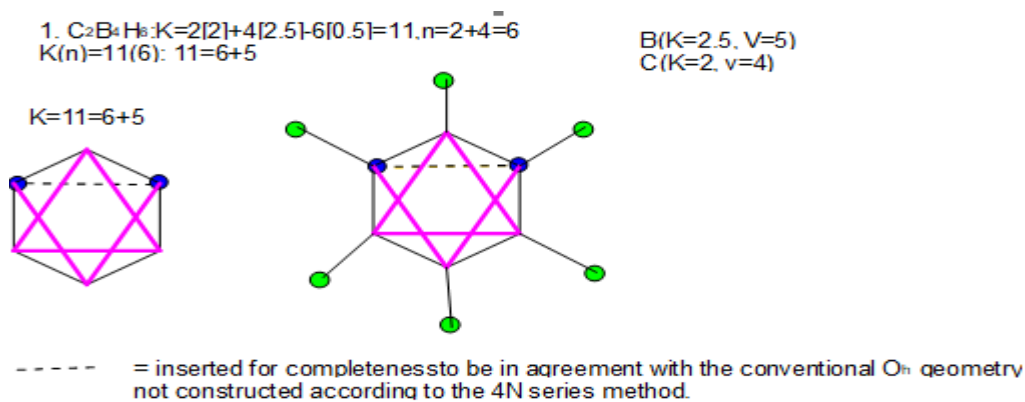


Figure 9. Isomeric graphical structure of $C_2B_4H_6$

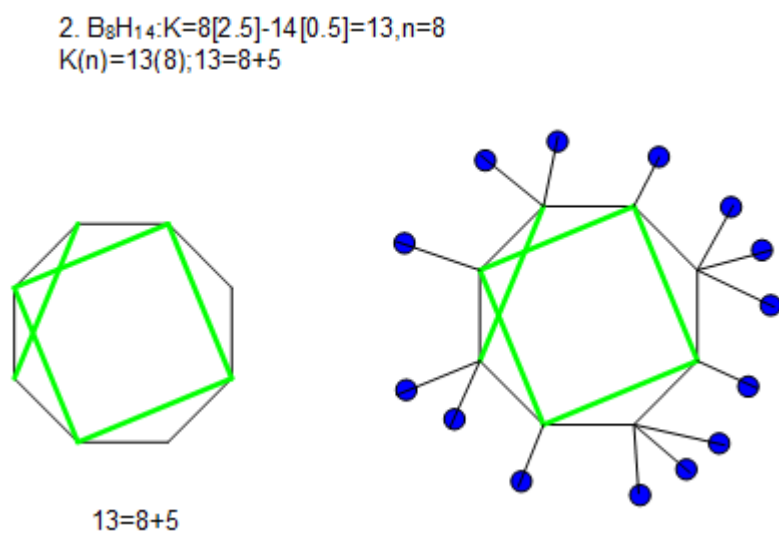


Figure 10. Isomeric graphical structure of B_8H_{14}

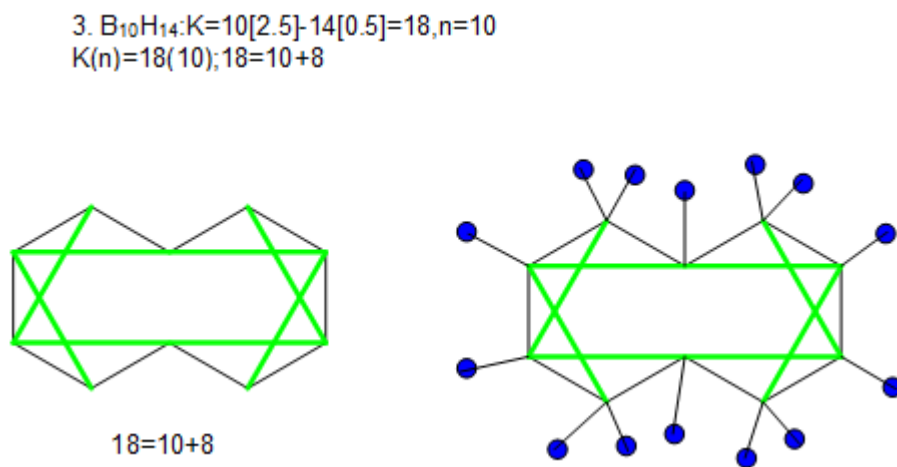


Figure 11. Isomeric graphical structure of $B_{10}H_{14}$

4. $C_2B_{10}H_{12}:K=2[2]+10[2.5]-12[0.5]=23, n=2+10=12$
 $K(n)=23(12):23=12+11$

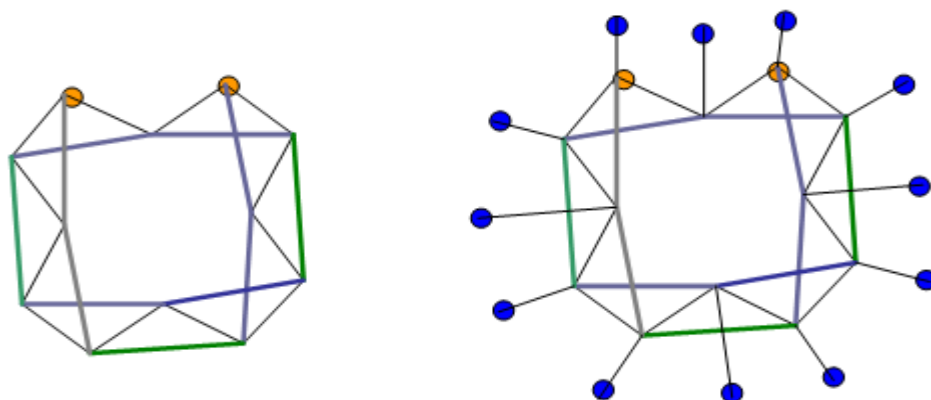


Figure 12. Isomeric graphical structure of $C_2B_{10}H_{12}$

5. $B_{12}=12[2.5]=30, n=12$
 $K(n)=30(12):30=12+18$

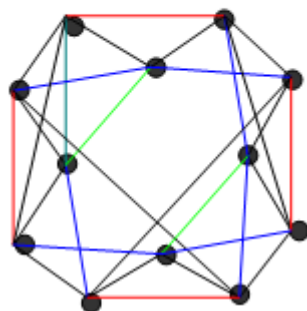
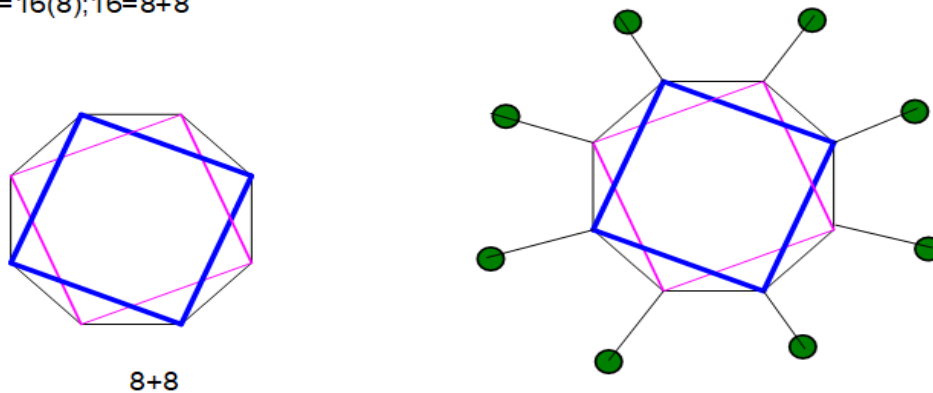


Figure 13. Isomeric graphical structure of B_{12}

6. $B_8Cl_8:K=8[2.5]-8[0.5]=16, n=8$
 $K(n)=16(8):16=8+8$



8+8

Figure 14. Isomeric graphical structure of $B_{12}Cl_8$

7. $B_9Cl_9: K=9[2.5]-9[0.5]=18, n=9$
 $K(n)=18(9); 18=9+9$

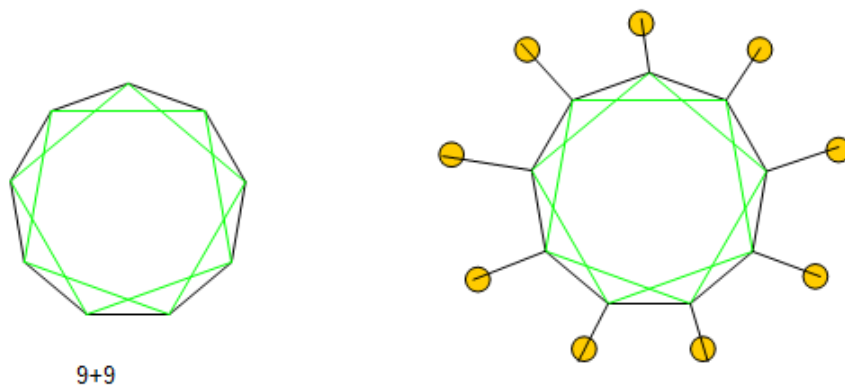


Figure 15. Isomeric graphical structure of B_9Cl_9

8. $B_{20}H_{26}: K=20[2.5]-13=37, n=20$
 $K(n)=37(20)$
 $2[20]-37=3$
 $S=4n+6$
 $K=2n-3$
 $Kp=C^{-2}C[M22]$
 $K^*=C^{-2}+D^{22}$
 $\gamma=-2, z=22$
 $VE_0=2z+2=2[22]+2=46$
 $VE=VE_0+2n=46+2[20]=46+40=86$
 $VE=2\gamma+4z+2=2[-2]+4[22]+2=-4+88+2=86$
 $VF=20[3]+26=60+26=86$

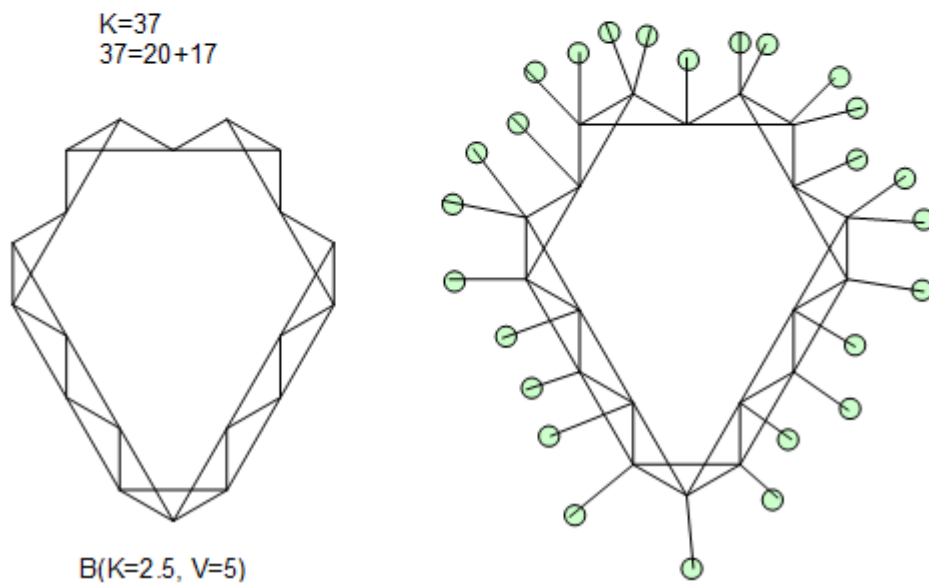


Figure 16. Isomeric graphical structure of $B_{20}H_{26}$

$$\begin{aligned}
 9. B_{20}H_{26}: K &= 20[2.5] - 13 = 37, n = 20 \\
 K(n) &= 37(20) \\
 2[20] - 37 &= 3 \\
 S &= 4n + 6 \\
 K &= 2n - 3 \\
 K_p &= C^{-2}C[M22] \\
 K^* &= C^{-2} + D^{22} \\
 y &= 2, z = 22 \\
 VE_0 &= 2z + 2 = 2[22] + 2 = 46 \\
 VE &= VE_0 + 2n = 46 + 2[20] = 46 + 40 = 86 \\
 VE &= 2y + 4z + 2 = 2[-2] + 4[22] + 2 = -4 + 88 + 2 = 86 \\
 VF &= 20[3] + 26 = 60 + 26 = 86
 \end{aligned}$$

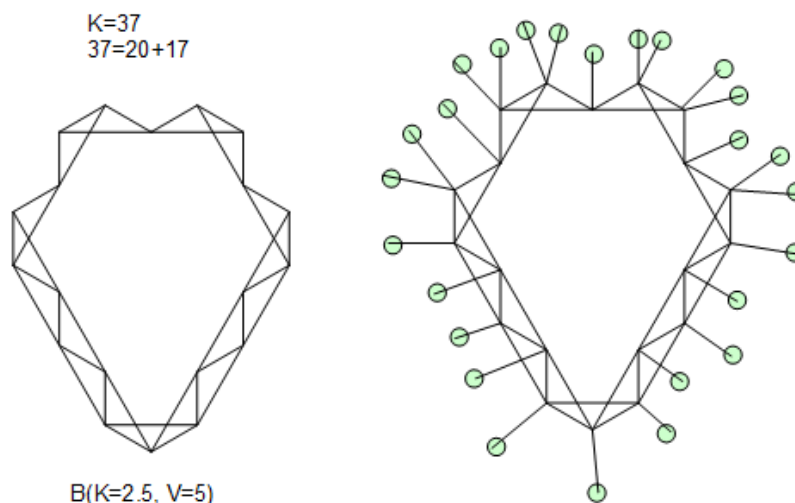


Figure 17. Isomeric graphical structure of $B_{20}H_{26}$

3. Categorization of Borane Clusters

A systematic method of categorization of clusters was recently developed (Kiremire 2019a-c). According to the method, a categorization parameter $K^* = C^y + D^z$ was introduced where $y+z=n$ = normally is number of skeletal elements in the cluster and C = represents the outer capping symbol and D represents the inner capping symbol of the cluster as it was discovered that clusters and chemical elements portray double capping phenomena. The symbol D^z is also regarded as representing CLAN series of the clusters (Kiremire, 2019a-c). The analyzed boranes fall within the range D^1 - D^{22} cluster clans and are shown in Table 1. The capping is in line with the descending cluster series that Rudolph identified more than 40 years ago (Rudolph, 1976).

3.1 The Evolution of Isomeric Polyhedral Geometries

During the analysis of borane clusters including the construction of clusters shapes with nuclearity index of 5 and above, it has been found helpful to utilize ring structures corresponding to the level of the nuclearity index. This means that for example B_5 clusters, a 5-membered ring is used, B_6 clusters, we use a 6-membered ring, B_7 , 7-membered ring, B_8 , 8-membered ring and so on. According to this approach, there is a relationship between the cluster skeletal linkages K and the number of skeletal elements, n . This relationship is given between by $K=n+x$ where x =number of skeletal lines or triangles constructed. As this relationship is considered very important, is being repeated here for emphasis. Thus, for $K(n)=7(6)$, $7=6+1$ and therefore a 6-membered ring with one triangle constructed inside will fulfill the cluster valence content of all the hydrogen ligands in the cluster. This is the case for B_6H_{16} shown in Figure 18-0. The cluster B_6H_{14} with $K(n)=8(6)$; $8=6+2$, we will construct two triangles to be in resonance with the formula B_6H_{14} . This is shown in Figure 19. The procedure goes on for B_6H_{12} , $K(n)=9(6)$; $9=6+3 \rightarrow 3$ triangles; B_6H_{10} , $K(n)=10(6)$; $10=6+4 \rightarrow 4$ triangles, $B_6H_8[B_6H_6^{2-}] \rightarrow K(n)=11(6)$; $11=6+5 \rightarrow 5$ triangles, B_6H_6 , $K(n)=12(6)$; and $12=6+6 \rightarrow 6$ triangles. The increasing number of skeletal triangles are given in Figures 20-27. The $K(n)=12(6)$ value for B_6H_6 is the same as that of C_6 and $Os_6(CO)_{18}$. Therefore, these clusters have the same skeletal structure. These are shown in Scheme 1.

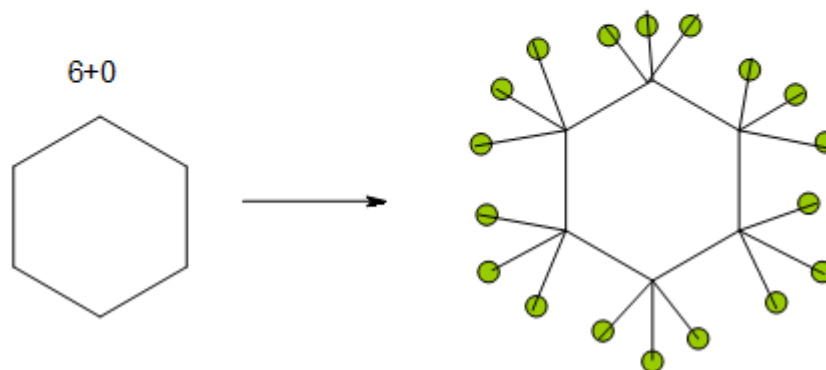
1.

$$B_6H_{18}: K=6[2.5]-18[0.5]=15-9=6, n=6$$

$$K(n)=6(6); 6=6+0$$

$$2[n]-K=2[6]-6=6, S=4n+12, K=2n-6, K_p=C^{-5}C[M11]_{\leftarrow}$$

$$K^*=C^{-5}+D^{11}_{\leftarrow}$$

Figure 18. Isomeric graphical structure of B_6H_{16}

$$2. F=B_6H_{16}: K=6[2.5]-8=7, n=6$$

$$K(n)=7(6)$$

$$2[6]-7=5$$

$$S=4n+10$$

$$K=2n-5$$

$$K_p=C^{-4}C[M10]$$

$$K^*=C^{-4}+D^{10}$$

$$y=-4, z=10$$

$$VE_0=2z+2=2[10]+2=22$$

$$VED_z=4z+2=4[10]+2=42$$

$$VE=VE_0+2n=22+2[6]=22+12=34$$

$$VF=6[3]+16=18+16=34$$

$$VE=VE_0+2y+2z=22+2[-4]+2[10]=34$$

$$VE=VED_z+2y=42+2[-4]=34$$

$$VE=2y+4z+2=2[-4]+4[10]+2=34$$

$$VE=8n-2K=8[6]-2[7]=34$$

$$VE=4n+10=4[6]+10=34$$

4. $B_6H_{14}: K=6[2.5]-7=8, n=6$
 $K(n)=8(6)$
 $2[6]-8=4$
 $S=4n+8$
 $K=2n-4$
 $K_p=C^{-3}C[M9]$
 $K^*=C^{-3}+D^9$
 $\gamma=-3, z=9$
 $VE_0=2z+2=2[9]+2=20$
 $VE=VE_0+2n=20+2[6]=32$
 $VE=VE_0+2\gamma+2z=20+2[-3]+2[9]=32$
 $VE=2\gamma+4z+2=2[-3]+4[9]+2=32$
 $VEDz=4z+2=4[9]+2=38$
 $VE=VEDz+2\gamma=38+2[-3]=32$
 $VE=8n-2K=8[6]-2[8]=32$
 $VE=4n+8=4[6]+8=32$
 $VF=6[3]+14=32$

B_6H_{14}
 $K=8$
 $B(K=2.5, V=5)$

$K(n)=8(6) \quad 8=6+2$

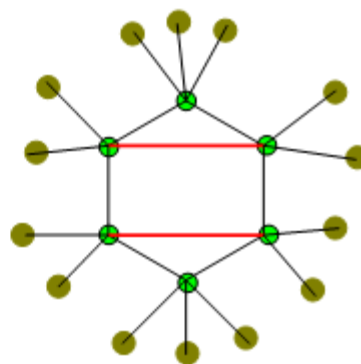
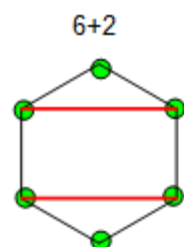
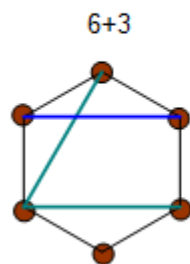


Figure 19. Isomeric graphical structure of B_6H_{14}

5. $B_6H_{12}: K=6[2.5]-6=9, n=6$
 $K(n)=9(6)$
 $9=6+3$



$K=9$
 $B(K=2.5, V=5)$

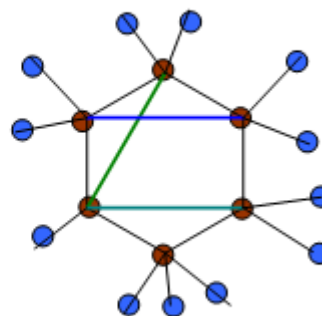


Figure 20. Isomeric graphical structure of B_6H_{12}

6. B_6H_{10} : $K=6[2.5]-5=10, n=6$
 $K(n)=10(6)$
 $10=6+4$

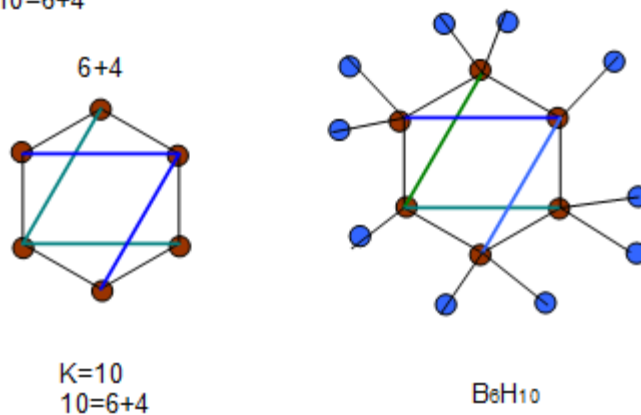


Figure 21. Isomeric graphical structure of B_6H_{10}

7. B_6H_8 : $K=6[2.5]-4=11, n=6$
 $K(n)=11(6)$
 $11=6+5$

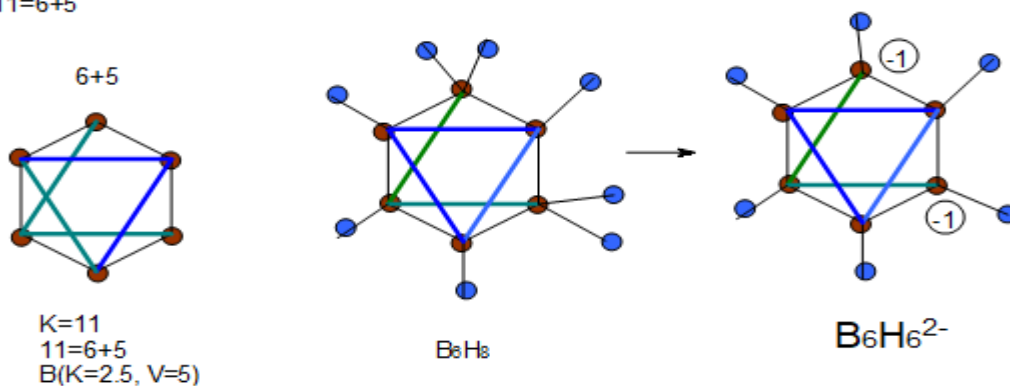
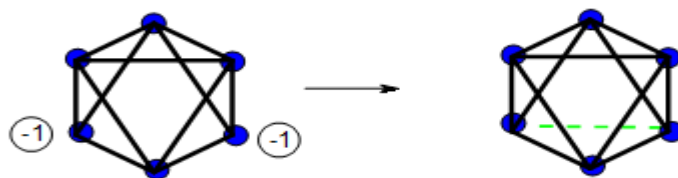


Figure 22. Isomeric graphical structure of B_6H_8



Linking up the nodal charges to get a closed shape

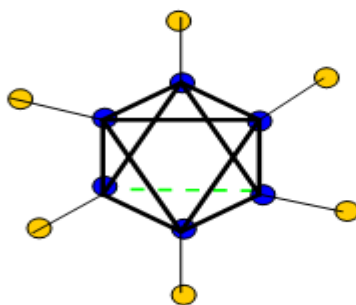
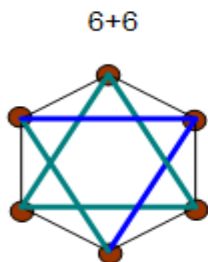


Figure 23. Isomeric graphical structure of $B_6H_6^{2-}$

As H Ligands Decrease, K Increases and More Triangles Are Formed.

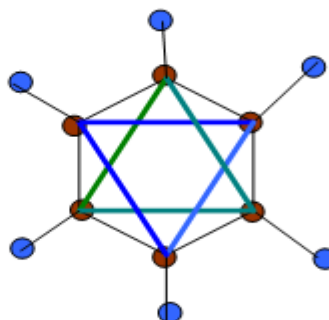
3.2 Closo Capping Series

8. $B_6H_6: K=6[2.5]-3=12, n=6$
 $K(n)=12(6)$
 $12=6+6$



$K=12$
 $12=6+6$
 $B(K=2.5, V=5)$

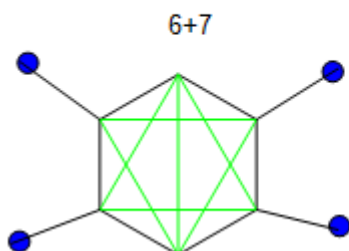
$K(n)=12(6), S=4n+0$
 $K_p=C^1C[M5]$
 $K^*=C^1+D^5$
 Mono-capped trigonal bipyramid shape



B_6H_6

Figure 24. Isomeric graphical structure of B_6H_6

$B_6H_4: K=6[2.5]-2=13, n=6$
 $K(n)=13(6); 13=6+7$

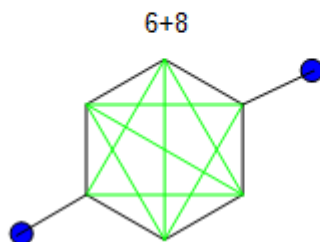


$K(n)=13(6)$
 $2[6]-13=-1$
 $S=4n-2$
 $K=2n+1$
 $K_p=C^2C[M4]$
 $K^*=C^2+D^4$

Bi-capped tetrahedral shape

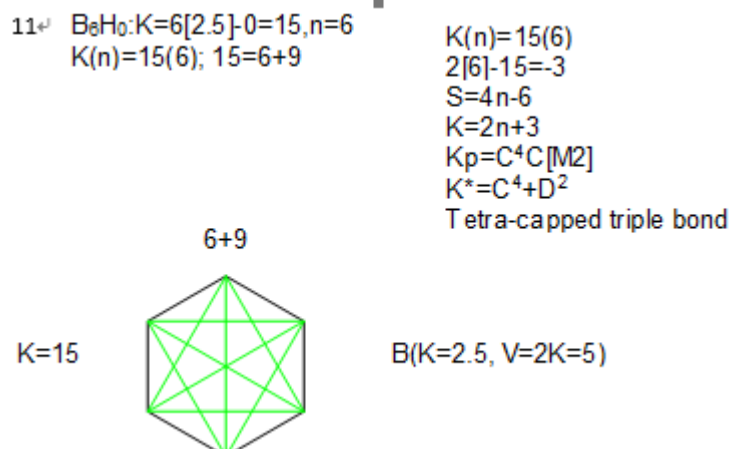
Figure 25. Isomeric graphical structure of B_6H_4

$B_6H_2: K=6[2.5]-1=14, n=6$
 $K(n)=14(6); 13=6+8$

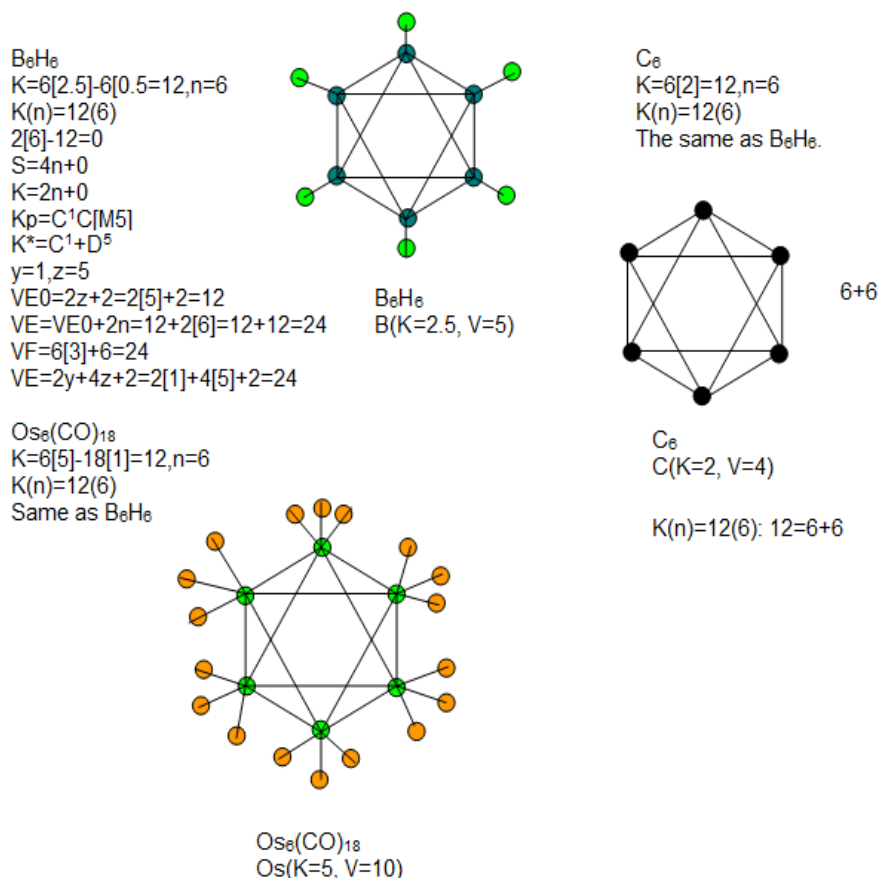


$K(n)=14(6)$
 $2[6]-14=-2$
 $S=4n-4$
 $K=2n+2$
 $K_p=C^3C[M3]$
 $K^*=C^3+D^3$
 Tri-capped triangle shape

Figure 26. Isomeric graphical structure of B_6H_2

Figure 27. Isomeric graphical structure of $B_6H_0 = B_6$

3.3 Equivalent Isomeric Skeletal Mono-Capping Clusters

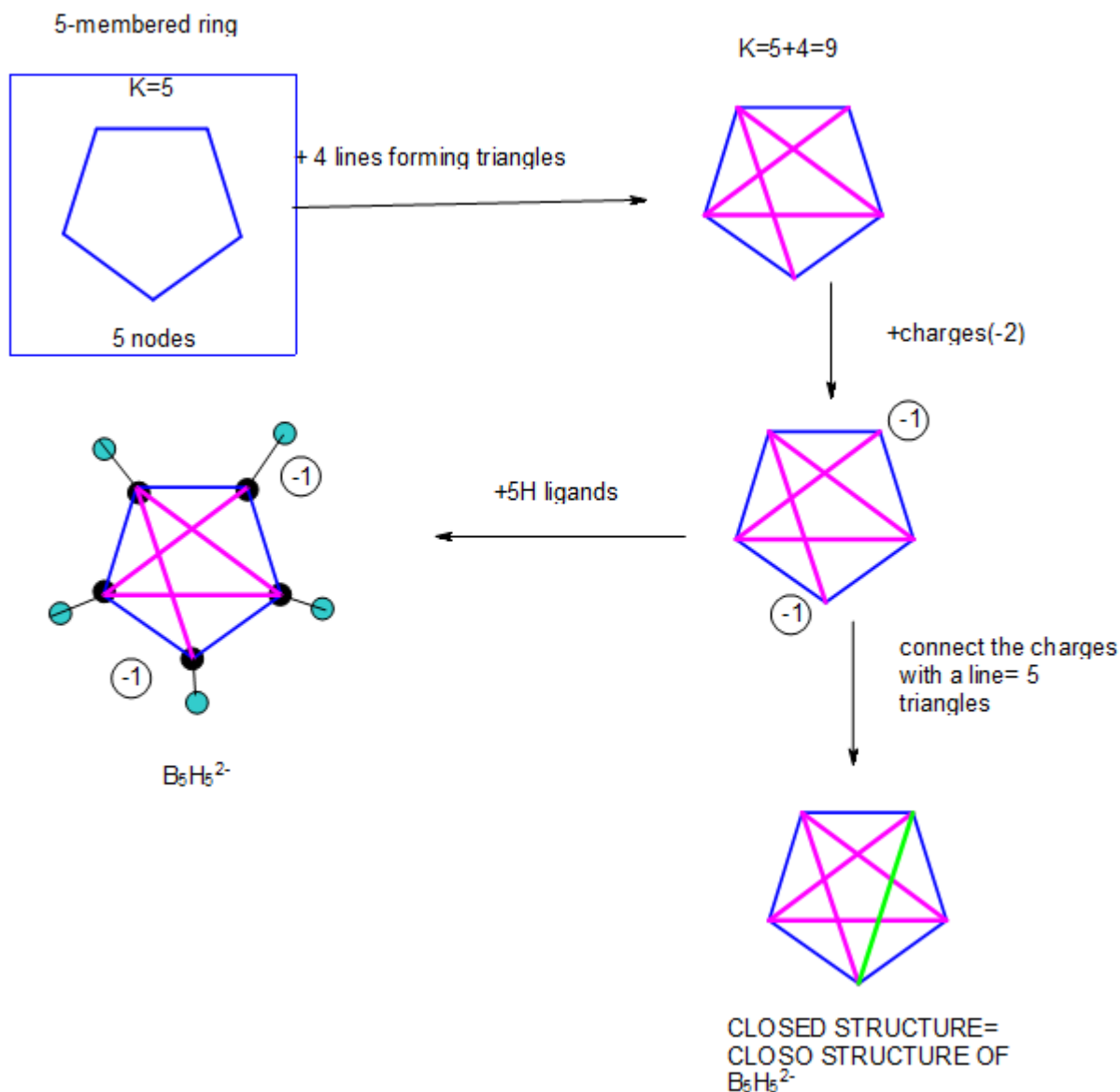
Scheme 1. Equivalent Isomeric graphical mono-capped closo structures of B_6H_6 , C_6 and $Os_6(CO)_{18}$

Since B_6H_6 , C_6 and $Os_6(CO)_{18}$ have the same $K(n)$ value, we can regard them as being equivalent SKELETAL ISOMERS. Since the CO ligand is a two-electron donor, it can be considered as using up 2 skeletal linkages of osmium skeletal element. The carbon skeletal element has 4 skeletal linkages which are all utilized in forming the isomeric skeletal structure of C_6 .

3.4 The Closo Series: $B_nH_n^{2-}$

The construction of the closo structures is similar to the general one of constructing other non-closo structures. The guidance is simply the $K(n)$ parameter of the cluster. First, an n -sided ring is selected. Then additional linkages are added

to the ring in such a way that the total linkages are the same as the numerical number of skeletal linkages K . That is, $K=n+x$ where x represents the number of additional linkages constructed in such a way that triangles are created including the nodal points carrying the negative charges. This procedure is shown in Scheme 2 for the closo $B_5H_5^{2-}$. In closo structures, the points with negative charges are linked by a line sealing off a triangle. The closo structures of selected boranes B_5-15 , B_{19-20} are given Figures 28 and 29.



Scheme 2. Construction of the formation of a closo structure of $B_5H_5^{2-}$

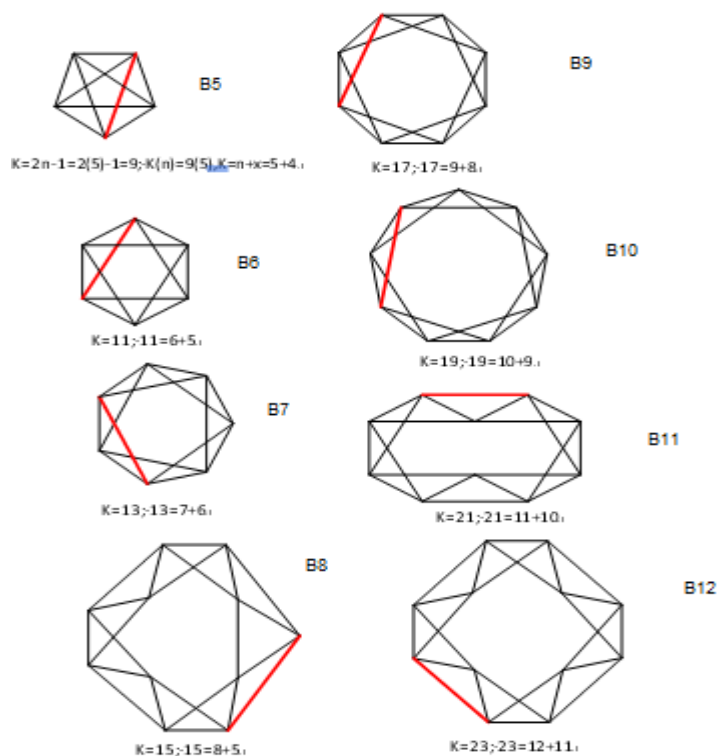


Figure 28. Closo isomeric structures of B₅ to B₁₂

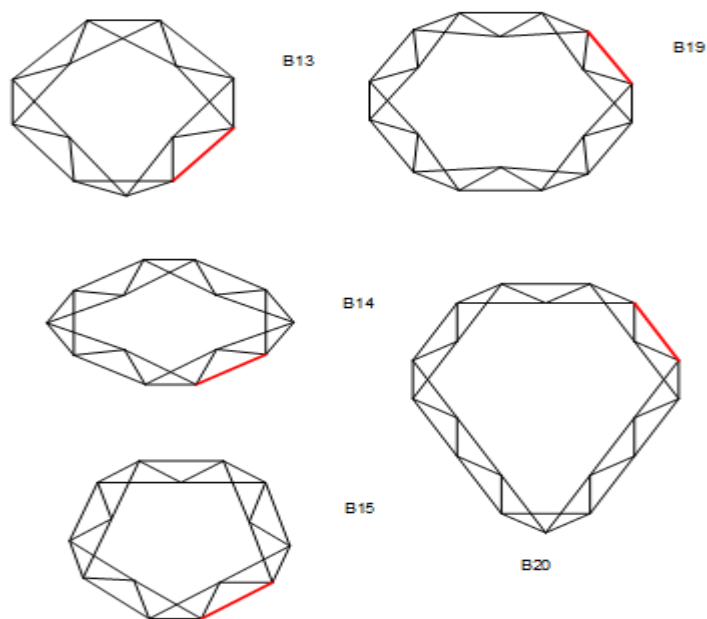


Figure 29. Isomeric graphical structure of B₁₃ to B₁₅, B₁₉-B₂₀

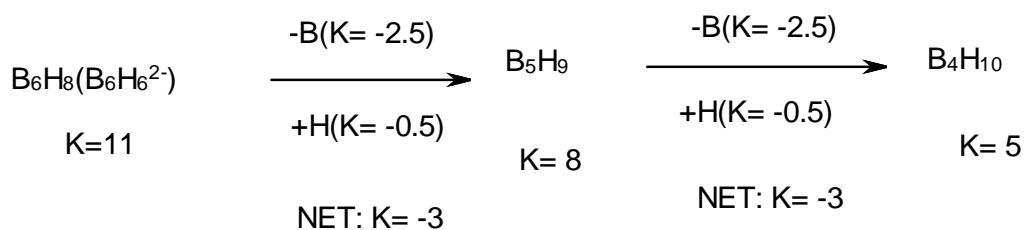
4. Descending Borane Clan Series (Dⁿ)

4.1 General Descending Series

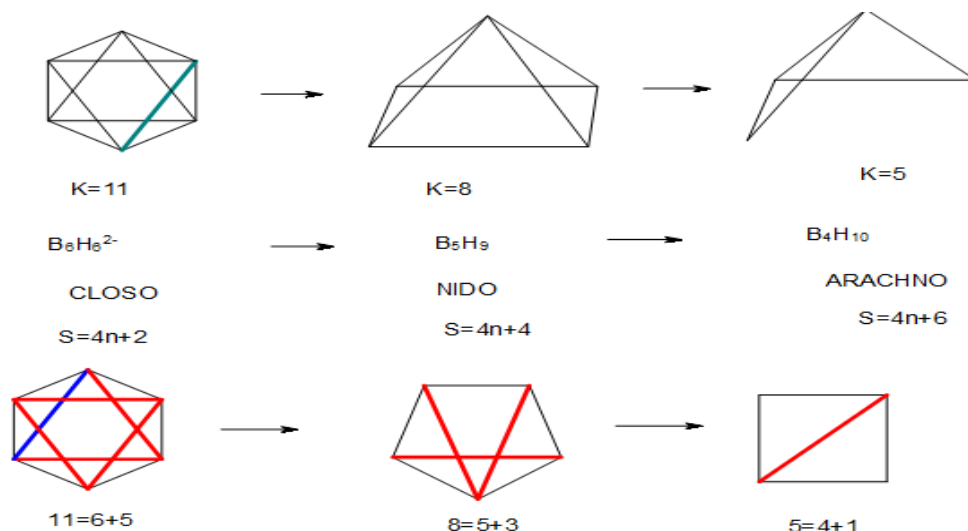
A wide range of clusters have been categorized into clan series using skeletal numbers. More than 60 borane clusters have been ranging from D⁵ to D²². Their analysis is given examples 1-51 some of their isomeric graphical shapes in Figures 1-54 and are presented in Table 1.

4.2 The popular Rudolph Clan Series

Clusters have broadly been categorized (Kiremire,2018). Those which change by $\Delta K = \pm 3$ and $\Delta n = \pm 1$ are in line with the cluster relationship which was brilliantly identified by Rudolph more than 40 years ago (Rudolph,1976).

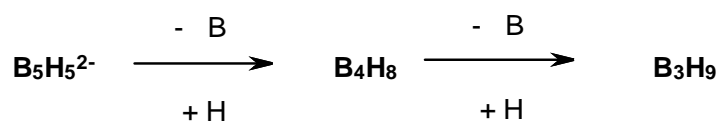


The Rudolph clan series behave as if a boron (B) skeletal element is transmuted into a hydrogen(H) ligand at each descending step. Also, a closo skeletal structure is obtained when the NODAL points bearing negative charges are linked up to generate an additional triangular face. The changes in the skeletal structure are shown in Scheme 3.



Scheme 3. Isomeric graphical structures of $B_6H_6^{2-}$, $B_5H_9^-$, B_4H_{10}

D⁵ SERIES



$$11. F=B_3H_5^{2-}:K=5[2.5]-5[0.5]-2[0.5]=9,n=5$$

$$K(n)=9(5)$$

$$10-9=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M5]$$

$$K^*=C^0+D^5$$

$$y=0, z=5$$

$$VE_0=2z+2=2[5]+2=12$$

$$VE=VE_0+2n=12+2[5]=22$$

$$VE=4n+2=4[5]+2=22$$

$$VF=5[3]+5+2=22$$

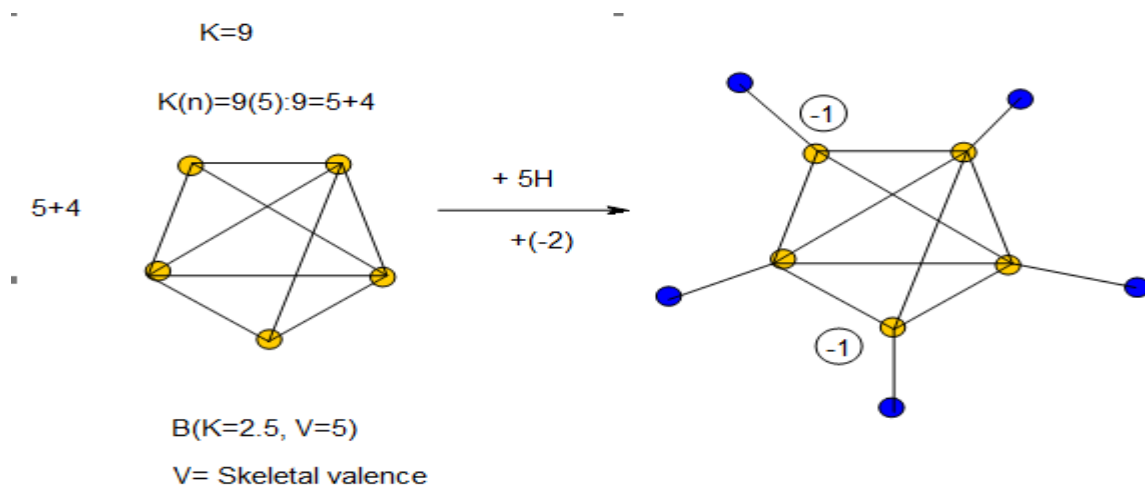


Figure 30. Isomeric graphical structure of $B_5H_5^{2-}$

12. $F=B_4H_8:K=4[2.5]-8[0.5]=6, n=4$

$K(n)=6(4)$

$8-6=2$

$S=4n+4(\text{nido})$

$K=2n-2$

$K_p=C^{-1}C[M5]$

$K^*=C^{-1}+D^5$

$y=-1, z=5$

$VE_0=2z+2=2[5]+2=12$

$VE=VE_0+2n=12+2[4]=12+8=20$

$VF=4[3]+8=20$

$VE=4n+4=4[4]+4=20$

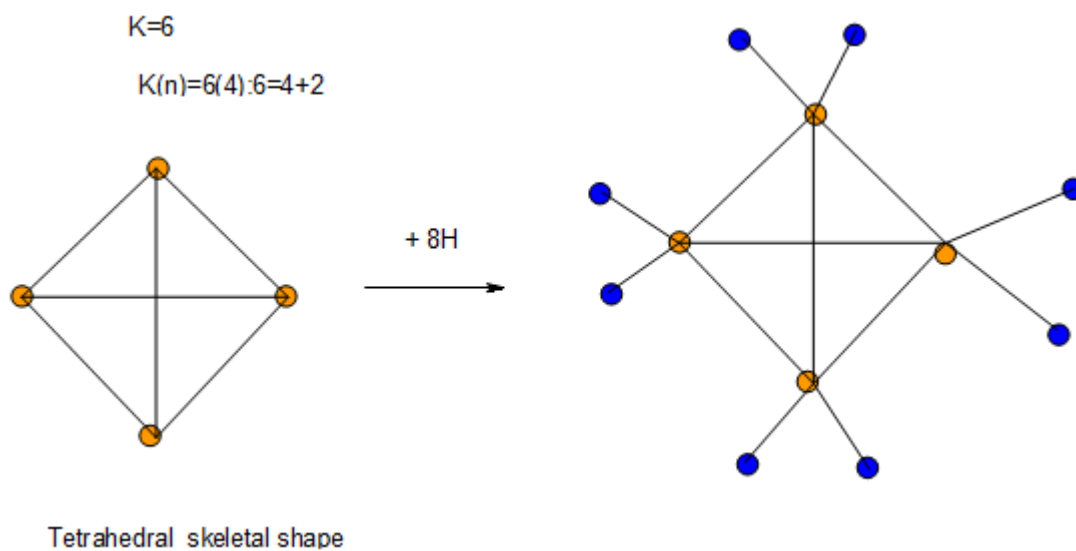


Figure 31. Isomeric graphical structure of B_4H_8

$$13. B_3H_9 \{K=3\}2.5]-9[0.5=3, n=3$$

$$K(n)=3(3)$$

$$6-3=3$$

$$S=4n+6(\text{arachno})$$

$$K=2n-3$$

$$K_p=C^{-2}C[M5]$$

$$K^*=C^{-2}+D^5$$

$$y=-2, z=5$$

$$VE_0=2z+2=2[5]+2=12$$

$$VED_z=4z+2=4[5]+2=22$$

$$VE=VE_0+2n=12+2[3]=12+6=18$$

$$VE=4n+6=4[3]+6=12+6=18$$

$$VF=3[3]+9=9+9=18$$

$$VE=VED_z+2y=22+2[-2]=18$$

$$VE=8n-2K=8[3]-2[3]=24-6=18$$

$$VE=VE_0+2y+2z=12+2[-2]+2[5]=12-4+10=18$$

$$VE=2y+4z+2=2[-2]+4[5]+2=22-4=18$$

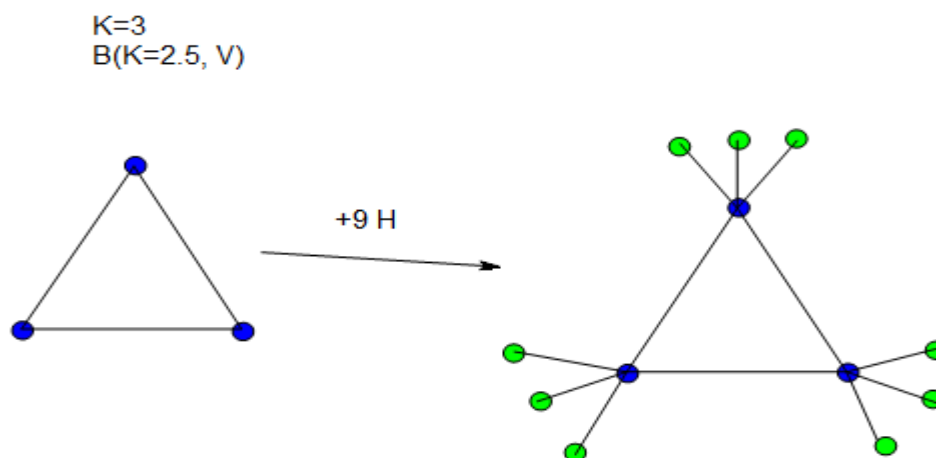


Figure 32. Isomeric graphical structure of B_3H_9

D^6 SERIES

$$14. F=B_6H_6^{2-}: K=6[2.5]-6[0.5]-2[0.5]=11, n=6$$

$$K(n)=11(6)$$

$$12-11=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M6]$$

$$K^*=C^0+D^6$$

$$y=0, z=6$$

$$VE_0=2z+2=2[6]+2=14$$

$$VED_z=4z+2=4[6]+2=26$$

$$VE=8n-2K=8[6]-2[11]=48-22=26$$

$$VE=4n+2=4[6]+2=26$$

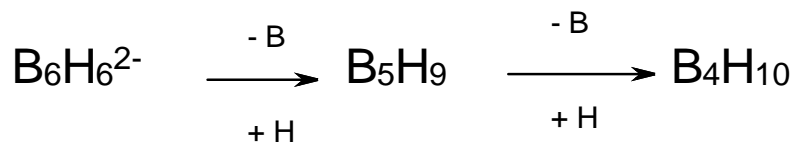
$$VE=6[3]+6+2=18+6+2=26$$

$$VE=VEDz+2y=26+2[0]=26$$

$$VE=2y+4z+2=2[0]+4[6]+2=26$$

$$VE=VE0+2y+2z=14+2[0]+2[6]=14+12=26$$

$$VF=6[3]+6+2=18+6+2=26$$



$$15.B_5H_9:K=5[2.5]-9[0.5]=8, n=5$$

$$K(n)=8(5)$$

$$10-8=2$$

$$S=4n+4$$

$$K=2n-2$$

$$Kp=C^{-1}C[M6]$$

$$K^*=C^{-1}+D^6$$

$$y=-1, z=6$$

$$VE0=2z+2=2[6]+2=14$$

$$VEDz=4z+2=4[6]+2=26$$

$$VE=8n-2K=8[5]-2[8]=40-16=24$$

$$VE=4n+4=4[5]+4=24$$

$$VE=VE0+2n=14+2[5]=24$$

$$VE=VE0+2y+2z=14+2[-1]+2[6]=14-2+12=24$$

$$VE=2y+4z+2=2[-1]+4[6]+2=-2+24+2=24$$

K=8

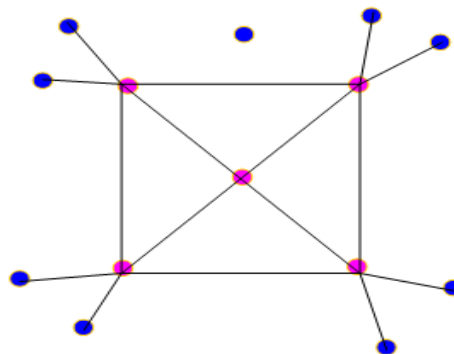
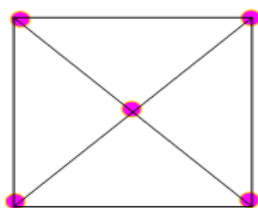


Figure 33. Isomeric graphical structure of B₅H₉

$$16. B_4H_{10}:K=4[2.5]-5=5, n=4$$

$$K(n)=5(4)$$

$$8-5=3$$

$$S=4n+6$$

$$K=2n-3$$

$$K_p=C^{-2}[M6]$$

$$K^*=C^{-2}+D^6$$

$$y=-2, z=6$$

$$VE_0=2z+2=2[6]+2=14$$

$$VED_z=4z+2=4[6]+2=26$$

$$VE=VE_0+2n=14+2[4]=22;$$

$$S=4n+6=4[4]+6=22$$

$$VE=8n-2K=8[4]-2[5]=32-10=22$$

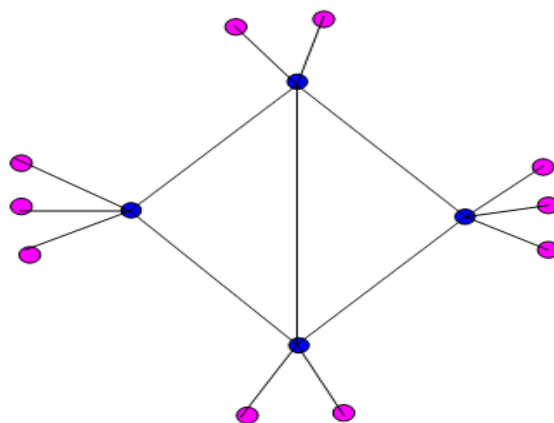
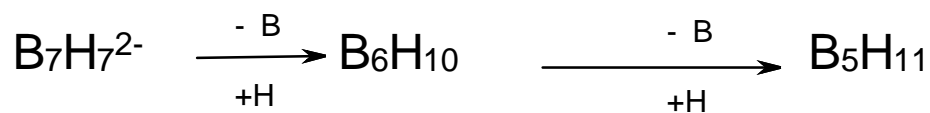


Figure 34. Isomeric graphical structure of B_4H_{10}

The structures in Figures 18 and 4 are skeletal isomers.

D⁷ SERIES



$$17. B_7H_7^{2-}:K=7[2.5]-7[0.5]-2[0.5]=13, n=7$$

$$K(n)=13(7)$$

$$14-13=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M7]$$

$$K^*=C^0+D^7$$

$$y=0, z=7$$

$$VE_0=2z+2=2[7]+2=16$$

$$VED_z=4z+2=4[7]+2=30$$

$$VE=8n-2K=8[7]-2[13]=56-26=30$$

$$VE=4n+2=4[7]+2=30$$

$$VE=VE_0+2n=16+2[7]=16+14=30$$

$$VF=7[3]+7+2=21+9=30$$

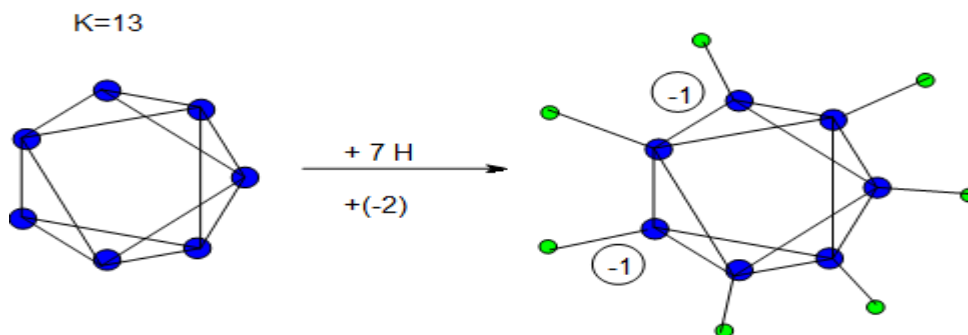


Figure 35. Isomeric graphical structure of $B_7H_7^{2-}$

$$18. B_6H_{10}:K=6[2.5]-10[0.5]=10, n=6$$

$$K(n)=10(6)$$

$$12-10=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C^{-1}C[M7]$$

$$K^*=C^{-1}+D^7$$

$$y=-1, z=7$$

$$VE_0=2z+2=2[7]+2=16$$

$$VE=VE_0+2n=16+2[6]=16+12=28$$

$$VE=4n+4=4[6]+4=24+4=28$$

$$VE=8n-2K=8[6]-2[10]=48-20=28$$

$$VF=6[3]+10=28$$

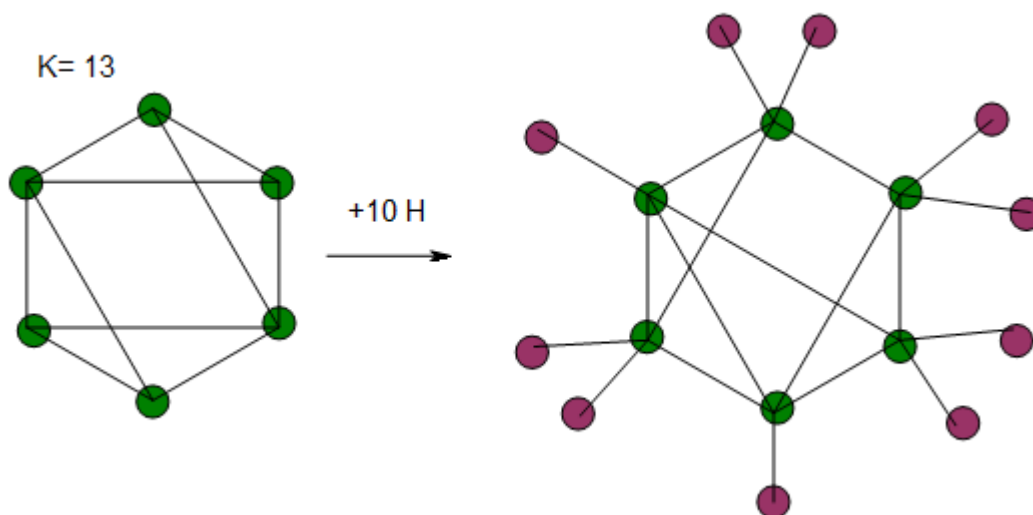


Figure 36. Isomeric graphical structure of B_6H_{10}

$$19. B_5H_{11}:K=5[2.5]-11[0.5]=7, n=5$$

$$K(n)=7(5)$$

$$10-7=3$$

$$S=4n+6(\text{arachno})$$

$$K=2n-3$$

$$K_p=C^{-2}C[M7]$$

$$K^*=C^{-2}+D^7$$

$$y=-2, z=7$$

$$VE_0=2z+2=2[7]+2=16$$

$$VE=VE_0+2n=16+2[5]=16+10=26$$

$$VE=8n-2K=8[5]-2[7]=40-14=26$$

$$VE=4n+6=4[5]+6=26$$

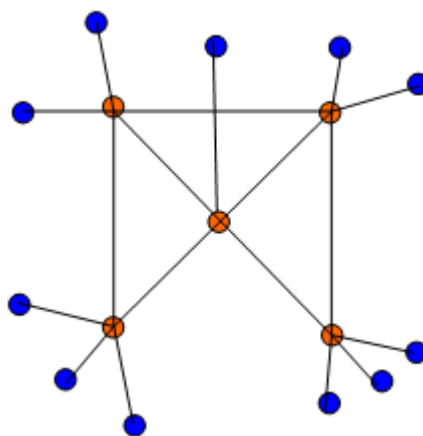


Figure 37. Isomeric graphical structure of B_5H_{11}

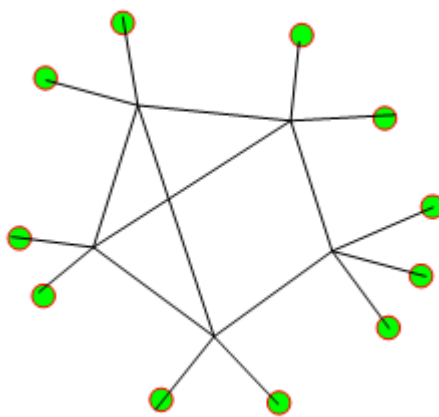
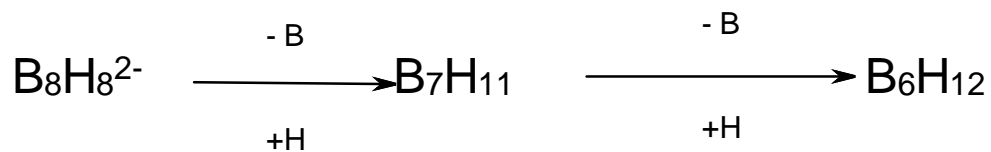


Figure 38. Isomeric graphical structure of B_5H_{11}

D⁸ SERIES



$$20. B_8H_8^{2-}: K=8[2.5]-8[0.5]-2[05]=15, n=8$$

$$K(n)=15(8)$$

$$16-15=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M8]$$

$$K^*=C^0+D^8$$

$$y=0, z=8$$

$$VE_0=2z+2=2[8]+2=18$$

$$VE=VE_0+2n=18+2[8]=18+16=34$$

$$VE=4n+2=4[8]+2=34$$

$$VF=8[3]+8+2=24+10=34$$

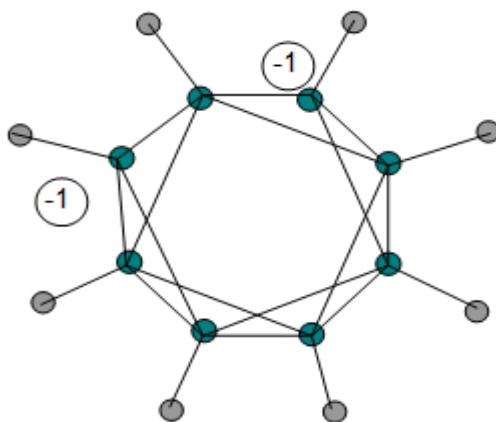


Figure 39. Isomeric graphical structure of $B_8H_8^{2-}$

$$21. B_7H_{11}: K=7[2.5]-11[0.5]=12, n=7$$

$$K(n)=12(7)$$

$$14-12=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C^{-1}C[M8]$$

$$K^*=C^{-1}+D^8$$

$$y=-1, z=8$$

$$VE_0=2z+2=2[8]+2=18$$

$$VE=4n+4=4[7]+4=32$$

$$VE=VE_0+2n=18+2[7]=18+14=32$$

$$VF=7[3]=11=21+11=32$$

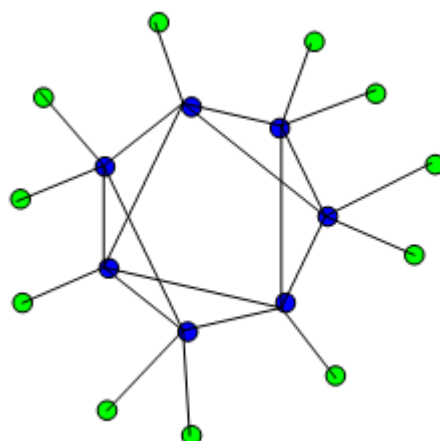


Figure 40. Isomeric graphical structure of B_7H_{11}

22. B_6H_{12} : $K=6[2.5]-6=9, n=6$

$K(n)=9(6)$

$12-9=3$

$S=4n+6(\text{arachno})$

$K=2n-3$

$K_p=C^{-2}C[M8]$

$K^*=C^{-2}+D^8$

$y=-2, z=8$

$VE_0=2z+2=2[8]+2=18$

$VE=VE_0+2n=18+2[6]=18+12=30$

$VE=8n-2K=8[6]-2[9]=48-18=30$

$VE=4n+6=4[6]+6=24+6=30$

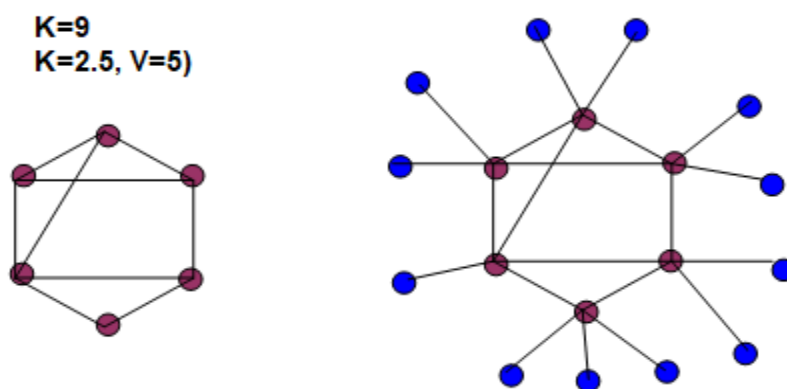
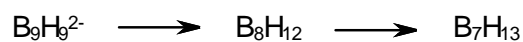


Figure 41. Isomeric graphical structure of B_6H_{12}

D⁹ SERIES



23. $K=9[2.5]-9[0.5]-2[0.5]=17, n=9$

$K(n)=17(9)$

$18-17=1$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M9]$$

$$K^*=C^0+D^9$$

$$y=0, z=9$$

$$VE_0=2z+2=2[9]+2=20$$

$$VE=VE_0+2n=20+2[9]=38$$

$$VE=4n+2=4[9]+2=38$$

$$VF=9[3]+9+2=27+9+2=27+11=38$$

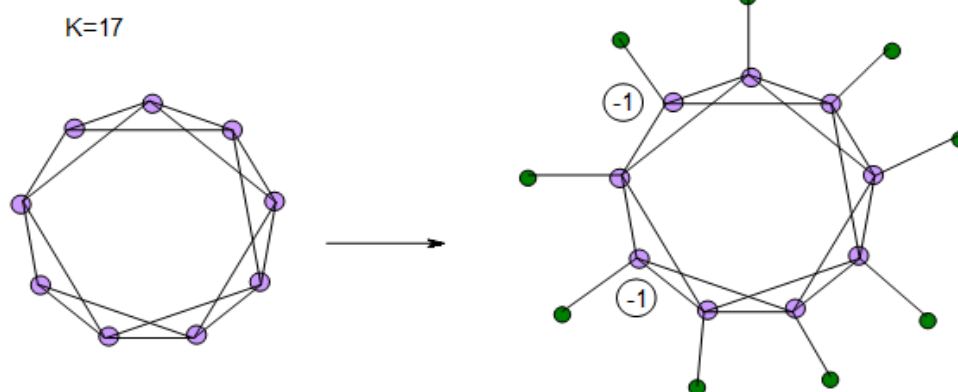


Figure 42. Isomeric graphical structure of $B_9H_9^{2-}$

$$24.B_8H_{12}:K=8[2.5]-6=14, n=8$$

$$K(n)=14(8)$$

$$16-14=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C^{-1}C[M9]$$

$$K^*=C^{-1}+D^9$$

$$y=-1, z=9$$

$$VE_0=2z+2=2[9]+2=20$$

$$VE=VE_0+2n=20+2[8]=20+16=36$$

$$VE=8n-2K=8[8]-2[14]=64-28=36$$

$$VE=4n+4=4[8]+4=32+4=36$$

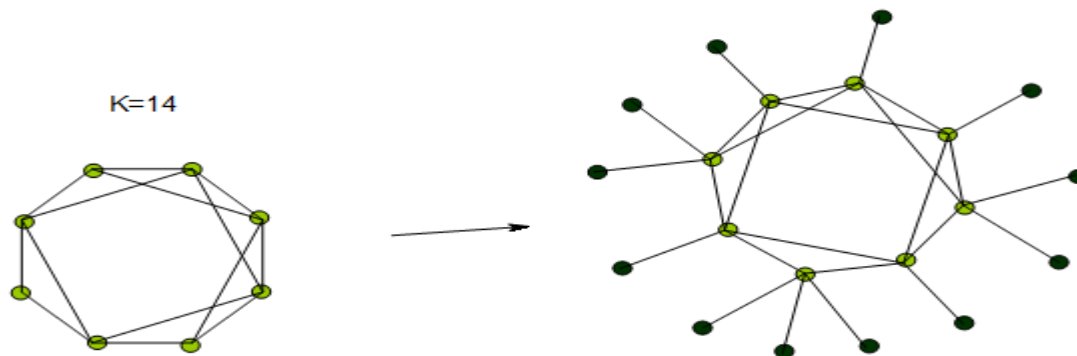


Figure 43. Isomeric graphical structure of B_8H_{12}

$$25. B_7H_{13}; K=7[2.5]-13[0.5]=11, n=7$$

$$K(n)=11(7)$$

$$14-11=3$$

$$S=4n+6(\text{arachno})$$

$$K=2n-3$$

$$K_p=C^{-2}C[M9]$$

$$K_p=C^{-2}+D^9$$

$$y=-2, z=9$$

$$VE_0=2z+2=2[9]+2=20$$

$$VE=VE_0+2n=20+2[7]=20+14=34$$

$$VE=8n-2K=8[7]-2[11]=56-22=34$$

$$VE=4n+6=4[7]+6=28+6=34$$

$$26. B_7H_{13}; K=7[2.5]-13[0.5]=11, n=7$$

$$K(n)=11(7)$$

$$14-11=3$$

$$S=4n+6(\text{arachno})$$

$$K=2n-3$$

$$K_p=C^{-2}C[M9]$$

$$K_p=C^{-2}+D^9$$

$$y=-2, z=9$$

$$VE_0=2z+2=2[9]+2=20$$

$$VE=VE_0+2n=20+2[7]=20+14=34$$

$$VE=8n-2K=8[7]-2[11]=56-22=34$$

$$VE=4n+6=4[7]+6=28+6=34$$

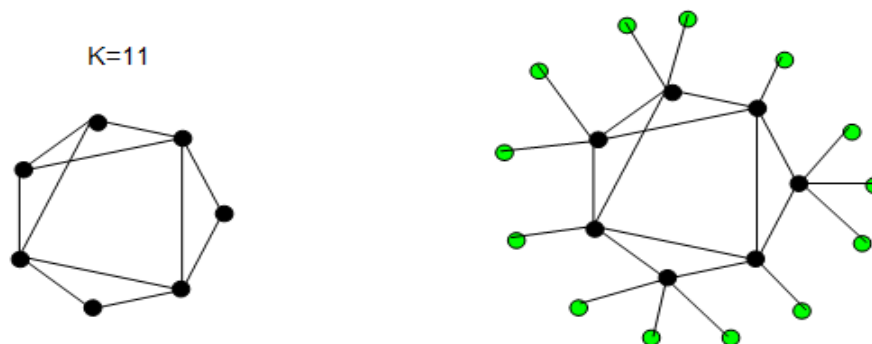
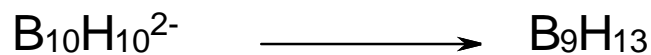


Figure 44. Isomeric graphical structure of B_7H_{13}

D^{10} SERIES



$$27. B_{10}H_{10}^{2-}; K=10[2.5]-5-1=19, n=10$$

$$K(n)=19(10)$$

$$20-19=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M10]$$

$$K^*=C^0+D^{10}$$

$$y=0, z=10$$

$$VE_0=2z+2=2[10]+2=22$$

$$VE=VE_0+2n=22+2[10]=22+20=42$$

$$VE=8n-2K=8[10]-2[19]=80-38=42$$

$$VE=4n+2=4[10]+2=42$$

$$VF=10[3]+10+2=42$$

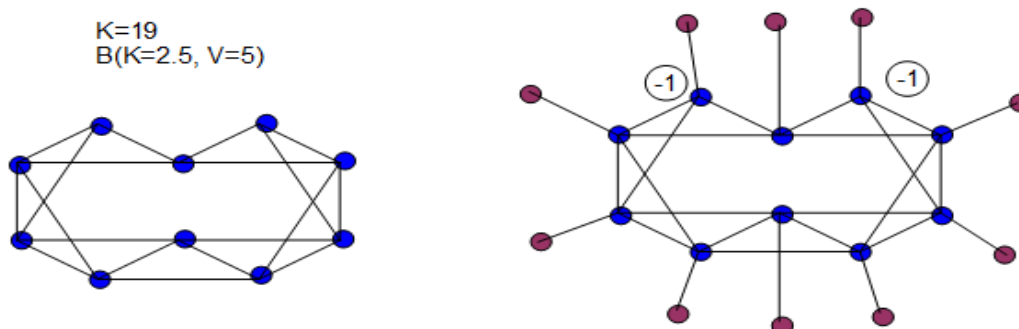


Figure 45. Isomeric graphical structure of $B_{10}H_{10}^{2-}$

$$28 B_9H_{13}:K=9[2.5]-13[0.5]=16, n=9$$

$$K(n)=16(9)$$

$$18-16=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C^{-1}C[M10]$$

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

$$y=-1, z=10$$

$$VE_0=2z+2=2[10]+2=22$$

$$VE=VE_0+2n=22+2[9]=22+18=40$$

$$VE=8n-2K=8[9]-2[16]=72-32=40$$

$$VE=4n+4=4[9]+4=36+4=40$$

$$VF=9[3]+13=27+13=40$$

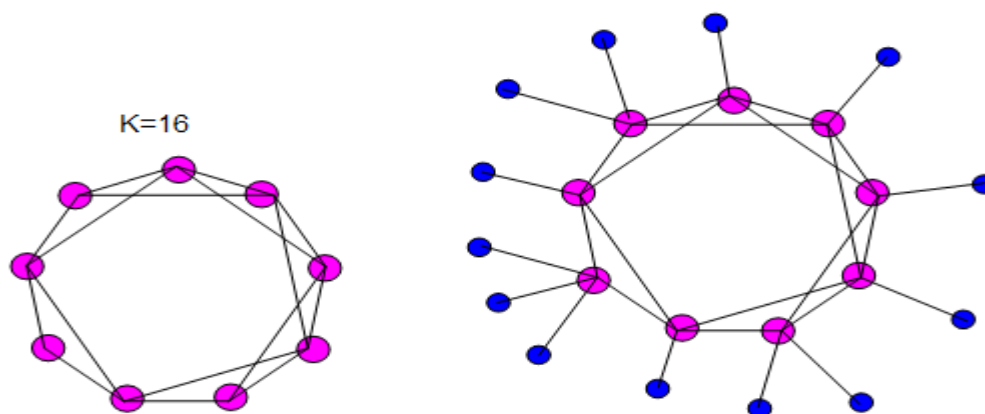


Figure 46. Isomeric graphical structure of B_9H_{13}

D¹¹ SERIES

$$29. B_{11}H_{11}^{2-}:K=11[2.5]-5.5-1=21, n=11$$

$$K(n)=21(11)$$

$$22-21=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M11]$$

$$K^*=C^0+D^{11}$$

$$y=0, z=11$$

$$VE_0=2z+2=2[11]+2=24$$

$$VE=VE_0+2n=24+2[11]=24+22=46$$

$$VE=8n-2K=8[11]-2[21]=88-42=46$$

$$VE=4n+2=4[11]+2=46$$

$$VF=11[3]+11+2=33+13=46$$

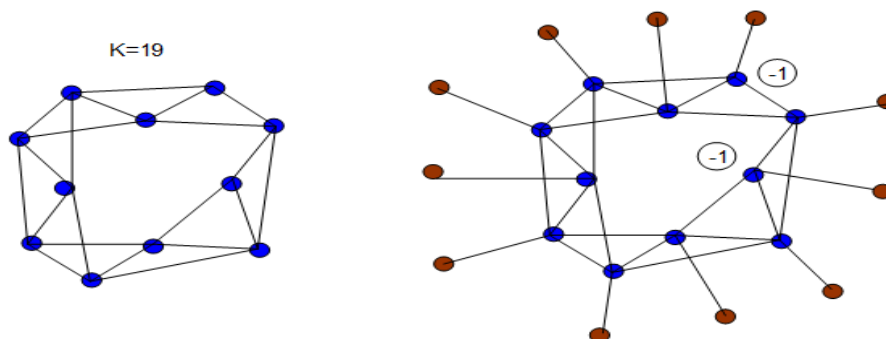


Figure 47. Isomeric graphical structure of $B_{11}H_{11}^{2-}$

$$30. B_{10}H_{14}:K=10[2.5]-7=18, n=10$$

$$K(n)=18(10)$$

$$20-18=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C^{-1}C[M11]$$

$$K^*=C^{-1}+D^{11}$$

$$y=-1, z=11$$

$$VE_0=2z+2=2[11]+2=24$$

$$VE=VE_0+2n=24+2[10]=24+20=44$$

$$VE=8n-2K=8[10]-2[18]=80-36=44$$

$$VE=4n+4=4[10]+4=44$$

$$VF=10[3]+14=44$$

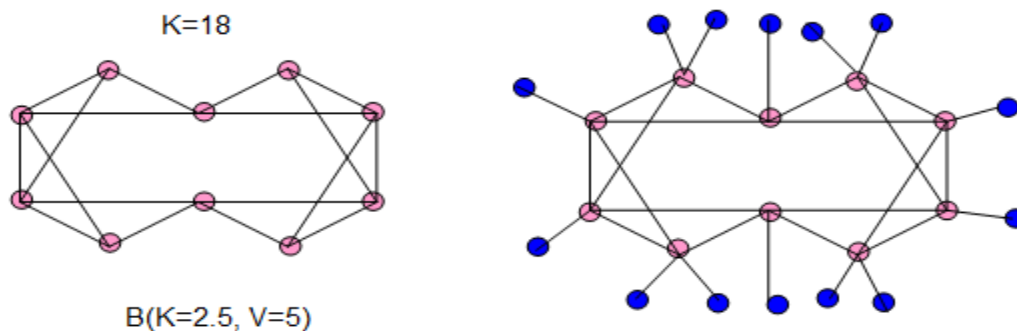
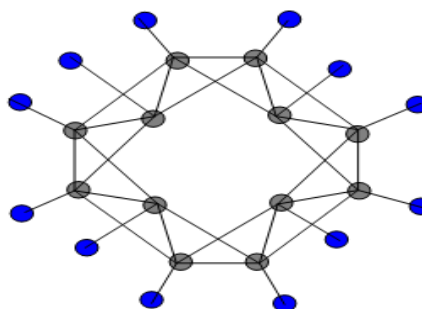
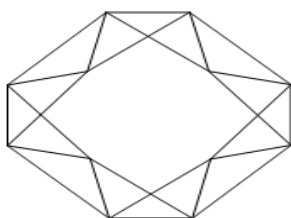


Figure 48. Isomeric graphical structure of $B_{10}H_{14}$

$$\begin{aligned}
 31.F=B_{12}H_{12}:K=24,n=12 \\
 K(n)=24(12) \\
 2[12]-24=0 \\
 S=4n+0 \\
 K=2n+0 \\
 Kp=C^1C[M11] \\
 K^*=C^1+D^{11} \\
 y=1, z=11 \\
 VE0=2z+2=2[11]+2=24 \\
 VE=VE0+2n=24+2[12]=24+24=48 \\
 VE=2y+4z+2=2[1]+4[11]+2=2+44+2=48 \\
 VF=12[3]+12=36+12=48
 \end{aligned}$$



$$\begin{aligned}
 K=24 \\
 24=12+12
 \end{aligned}$$

Figure 49. Isomeric graphical structure of $B_{12}H_{12}$

D¹² SERIES

$$32.B_{12}H_{12}^{2-}:K=12[2.5]-6-1=23,n=12$$

$$K(n)=23(12)$$

$$24-23=1$$

$$S=4n+2(\text{closes})$$

$$K=2n-1$$

$$Kp=C^0C[M12]$$

$$K^*=C^0+D^{12}$$

$$y=0,z=12$$

$$VE0=2z+2=2[12]+2=26$$

$$VE=VE0+2n=26+2[12]=26+24=50$$

$$VE=8n-2K=8[12]-2[23]=96-46=50$$

$$VE=4n+2=4[12]+2=50$$

$$VF=12[3]+12+2=36+14=50$$

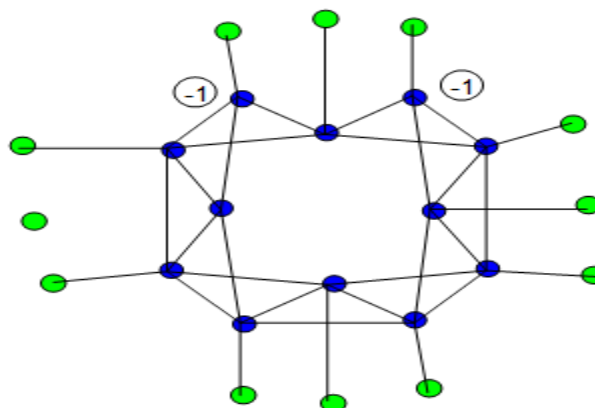
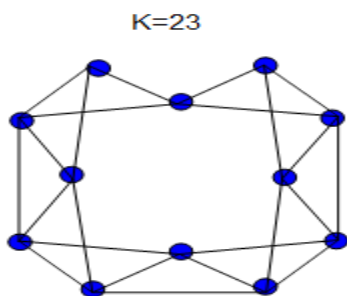


Figure 50. Isomeric graphical structure of $B_{12}H_{12}^{2-}$

$$33. B_{11}H_{15}:K=11[2.5]-15[0.5]=20,n=11$$

$$K(n)=20(11)$$

$$22-20=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C^{-1}C[M12]$$

$$K^*=C^{-1}+D^{12}$$

$$y=-1,z=12$$

$$VE_0=2z+2=2[12]+2=26$$

$$VE=VE_0+2n=26+2[11]=26+22=48$$

$$VE=8n-2K=8[11]-2[20]=88-40=48$$

$$VE=4n+4=4[11]+4=44+4=48$$

$$VF=11[3]+15=33+15=48$$

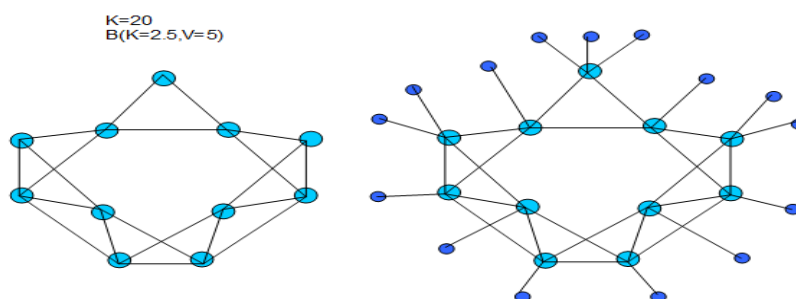


Figure 51. Isomeric graphical structure of $B_{11}H_{15}$

$$34. B_{10}H_{16}:K=10[2.5]-8=17,n=10$$

$$K(n)=17(10)$$

$$20-17=3$$

$$S=4n+6(\text{arachno})$$

$$K=2n-3$$

$$K_p=C^{-2}C[M12]$$

$$K^*=C^{-2}+D^{12}$$

$$y=-2,z=12$$

$$VE_0=2z+2=2[12]+2=26$$

$$VE=VE_0+2n=26+2[10]=46$$

$$VE=2y+4z+2=2[-2]+4[12]+2=-4+48+2=50-4=46$$

$$VF=10[3]+16=30+16=46$$

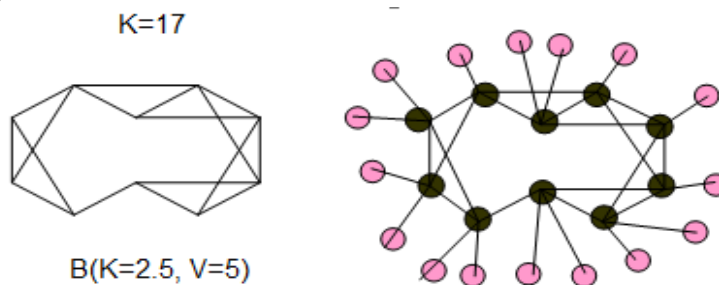


Figure 52. Isomeric graphical structure of $B_{10}H_{16}$

$$35. B_9H_{17}: K=9[2.5]-8.5=14, n=9$$

$$K(n)=14(9)$$

$$18-14=4$$

$$S=4n+8(\text{arachno})$$

$$K=2n-4$$

$$K_p=C^{-3}C[M12]$$

$$K^*=C^{-3}+D^{12}$$

$$y=-3, z=12$$

$$VE_0=2z+2=2[12]+2=26$$

$$VE=VE_0+2n=26+2[9]=26+18=44$$

$$VE=2y+4z+2=2[-3]+4[12]+2=-6+48+2=50-6=44$$

$$VF=9[3]+17=27+17=44$$

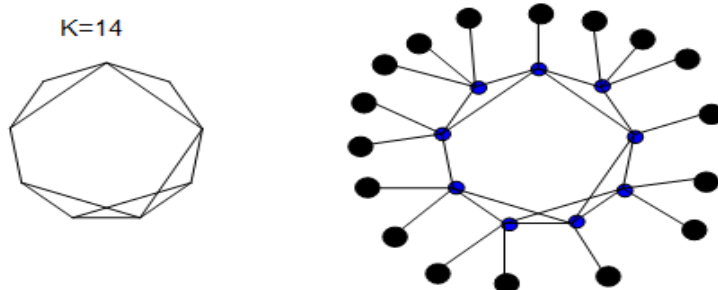


Figure 53. Isomeric graphical structure of $B_{13}H_{13}^{2-}$

$$36. B_8H_{18}: K=8[2.5]-9=11, n=8$$

$$K(n)=11(8)$$

$$16-11=5$$

$$S=4n+10(\text{klapo})$$

$$K=2n-5$$

$$K_p=C^{-4}C[M12]$$

$$K^*=C^{-4}+D^{12}$$

$$y=-4, z=12$$

$$VE=2y+4z+2=2[-4]+4[12]+2=-8+48+2=40+2=42$$

$$VE=8n-2K=8[8]-2[11]=64-22=42$$

$$VF=8[3]+18=24+18=42$$

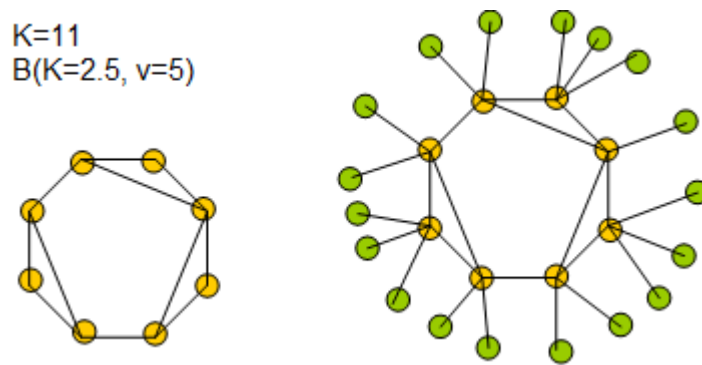


Figure 54. Isomeric graphical structure of B_8H_{18}

D¹³ SERIES

$$37. B_{13}H_{13}^{2-}: K=13[2.5]-6.5-1=25, n=13$$

$$K(n)=25(13)$$

$$26-25=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M13]$$

$$K^*=C^0+D^{13}$$

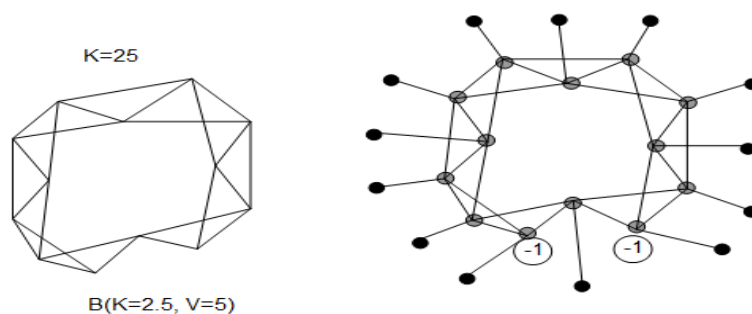
$$y=0, z=13$$

$$VE_0=2z+2=2[13]+2=28$$

$$VE=VE_0+2n=28+2[13]=28+26=54$$

$$VE=8n-2K=8[13]-2[25]=104-50=54$$

$$VE=4n+2=4[13]+2=54$$

Figure 55. Isomeric graphical structure of B_8H_{18}

$$38. B_{12}H_{16}: K=12[2.5]-8=22, n=12$$

$$K(n)=22(12)$$

$$24-22=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C-1C[M13]$$

$$K^*=C^{-1}+D^{13}$$

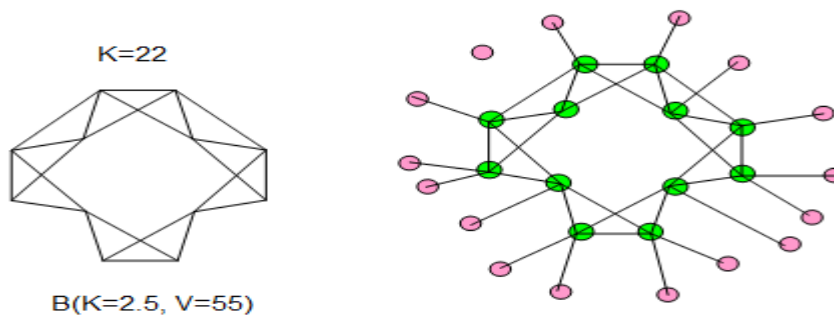
$$y=-1, z=13$$

$$VE_0=2z+2=2[13]+2=28$$

$$VE=VE_0+2n=28+2[12]=28+24=52$$

$$VE=8n-2K=8[12]-2[22]=96-44=52$$

$$VE=4n+4=4[12]+4=52$$

Figure 56. Isomeric graphical structure of $B_{12}H_{16}$

D¹⁴ SERIES

$$39. B_{14}H_{14}^{2-}: K=14[2.5]-7-1=27, n=14$$

$$K(n)=27(14)$$

$$28-27=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M14]$$

$$K^*=C^0+D^{14}$$

$$y=0, z=14$$

$$VE_0=2z+2=2[14]+2=30$$

$$VE=VE_0+2n=30+2[14]=30+28=58$$

$$VE=8n-2K=8[14]-2[27]=112-54=58$$

$$S=4n+2=4[14]+2=58$$

$$40. B_{13}H_{17}: K=13[2.5]-8.5=24, n=13$$

$$K(n)=24(13)$$

$$26-24=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C^{-1}C[M14]$$

$$K^*=C^{-1}+D^{14}$$

$$y=-1, z=14$$

$$VE_0=2z+2=2[14]+2=30$$

$$VE=VE_0+2n=30+2[13]=56$$

$$VE=8n-2K=8[13]-2[24]=56$$

$$VE=4n+4=4[13]+4=56$$

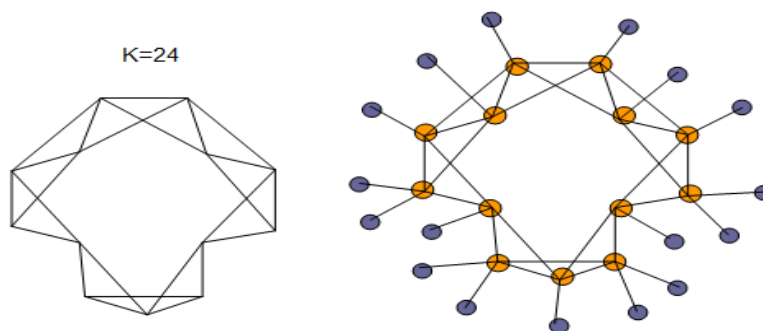


Figure 57. Isomeric graphical structure of $B_{13}H_{17}$

D¹⁵ SERIES

$$41. B_{15}H_{15}^{2-}: K=15[2.5]-7.5-1=29, n=15$$

$$K(n)=29(15)$$

$$30-29=1$$

$$S=4n+2(\text{closo})$$

$$K=2n-1$$

$$K_p=C^0C[M15]$$

$$K^*=C^0+D^{15}$$

$$y=0, z=15$$

$$VE_0=2z+2=2[15]+2=32$$

$$VE=VE_0+2n=32+2[15]=32+30=62$$

$$VE=8n-2K=8[15]-2[29]=120-58=62$$

$$VE=4n+2=4[15]+2=62$$

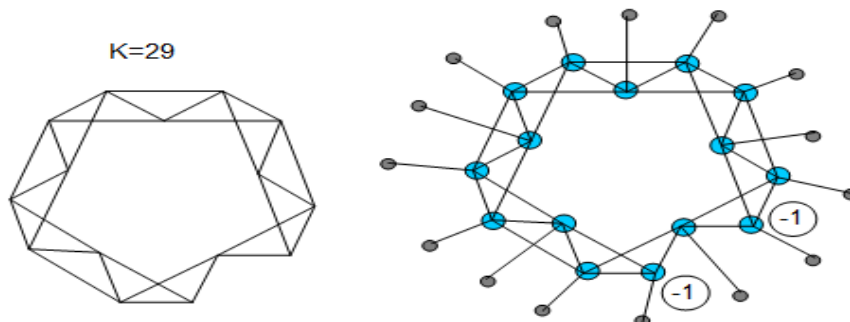


Figure 58. Isomeric graphical structure of $B_{15}H_{15}^{2-}$

$$42. B_{14}H_{18}: K=14[2.5]-9=26, n=14$$

$$K(n)=26(14)$$

$$28-26=2$$

$$S=4n+4(\text{nido})$$

$$K=2n-2$$

$$K_p=C^{-1}C[M15]$$

$$K^*=C^{-1}+D^{15}$$

$$y=-1, z=15$$

$$VE_0=2z+2=2[15]+2=32$$

$$VE=VE_0+2n=32+2[14]=32+28=60$$

$$VE=8n-2K=8[14]-2[26]=112-52=60$$

$$VE=4n+4=4[14]+4=60$$

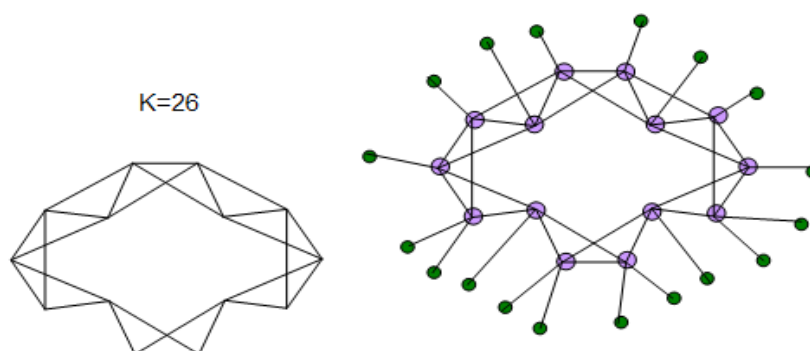


Figure 59. Isomeric graphical structure of $B_{14}H_{18}$

$$43. B_{13}H_{19}: K=13[2.5]-9.5=23, n=13$$

$$K(n)=23(13)$$

$$26-23=3$$

$$S=4n+6(\text{arachno})$$

$$K=2n-3$$

$$K_p=C^{-2}C[M15]$$

$$K^*=C^{-2}+D^{15}$$

$$y=-2, z=15$$

$$VE_0=2z+2=2[13]+2=28$$

$$VE=VE_0+2n=28+2[13]=28+26=54$$

$$44. B_{12}H_{20}: K=12[2.5]-10=20, n=12$$

$$K(n)=20(12)$$

$$24-20=4$$

$$S=4n+8(\text{hypho})$$

$$K=2n-4$$

$$K_p=C^{-3}C[M15]$$

$$K^*=C^{-3}+D^{15}$$

$$y=-3, z=15$$

$$VE_0=2z+2=2[15]+2=32$$

$$VE=VE_0+2n=32+2[12]=32+24=56$$

$$VF=12[3]+20=36+20=56$$

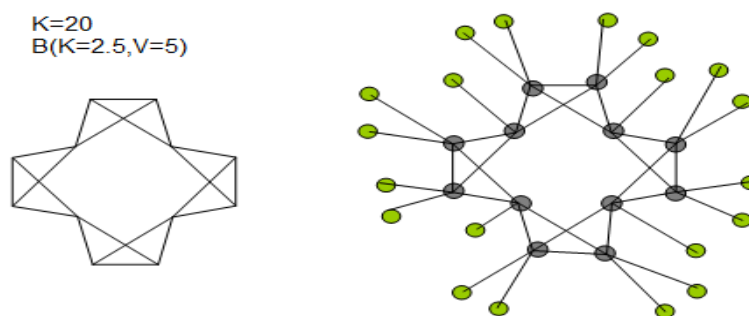


Figure 60. Isomeric graphical structure of $B_{12}H_{20}$

$$45. B_{11}H_{21}: K=11[2.5]-10.5=17, n=11$$

$$K(n)=17(11)$$

$$22-17=5$$

$$S=4n+10(\text{klapo})$$

$$K=2n-5$$

$$K_p=C^{-4}C[M15]$$

$$K^*=C^{-4}+D^{15}$$

$$y=-4, z=15$$

$$VE_0=2z+2=2[15]+2=32$$

$$VE=VE_0+2n=32+2[11]=32+22=54$$

$$VF=11[3]+21=33+21=54$$

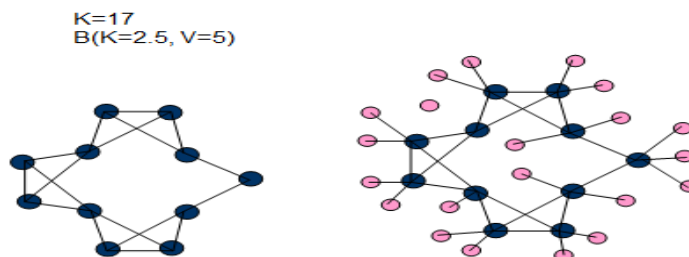


Figure 61. Isomeric graphical structure of $B_{11}H_{21}$

46. $B_{10}H_{22}$: $K=10[2.5]-11=14$, $n=10$

$K(n)=14(10)$

$20-14=6$

$S=4n+12(\text{klapo})$

$K=2n-6$

$K_p=C^{-5}C[M15]$

$K^*=C^{-5}+D^{15}$

$y=-5, z=15$

$VE_0=2z+2=2[15]+2=32$

$VE=VE_0+2n=32+2[10]=32+20=52$

$VF=10[3]+22=30+22=52$

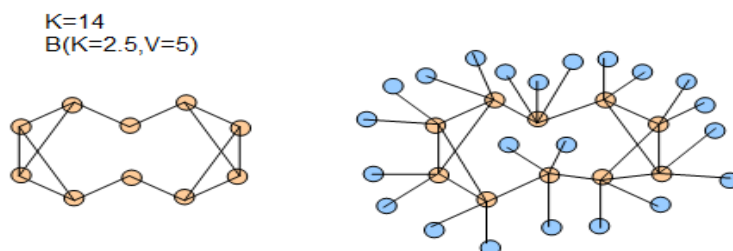


Figure 62. Isomeric graphical structure of $B_{10}H_{22}$

49. $B_{23}H_{19}$: $K=23[2.5]-19 [0.5] =48$, $n=23$

$K(n)=48(23)$

$2[23]-48=-2$

$S=4n-4$

$K=2n+2$

$K_p=C^3C[M20]$

$K^*=C^3+D^{20}$

$y=3, z=20$

$VE_0=2z+2=2 [20] +2 =42$

$VE=VE_0+2n=42+2 [23] =88$

$VED_z=4z+2=4 [20] +2=82$

$VE=VED_z+2y=82+2[3]=88$

$VE=2y+4z+2= 2[3] +4 [20] +2=88$

$VE=VE_0+2y+2z=42+2[3] +2 [20] =88$

$VE=8n-2K=8[23]-2 [48] =88$

$VE=4n-4=4[23]-4=88$

$VF=23 [3] + 19=88$

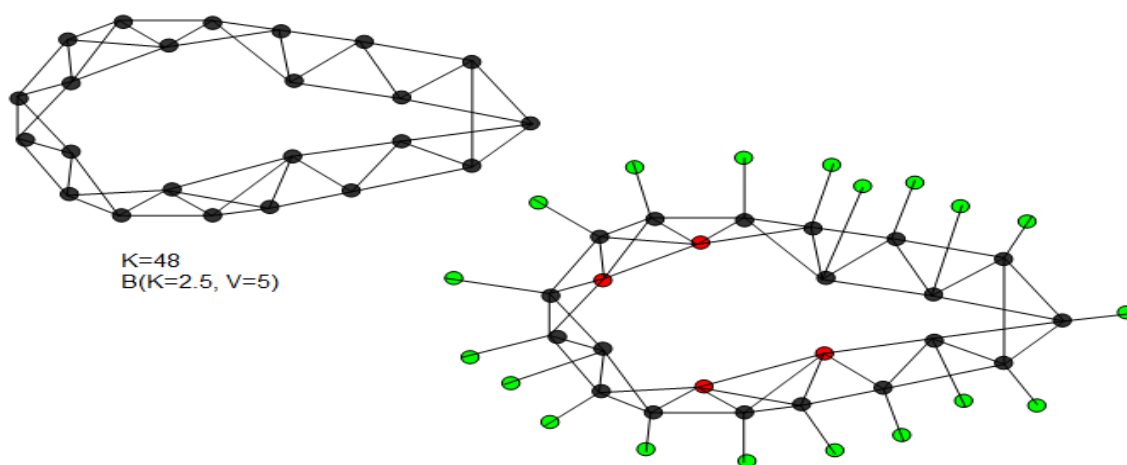


Figure 63. Isomeric graphical structure of $B_{23}H_{19}$

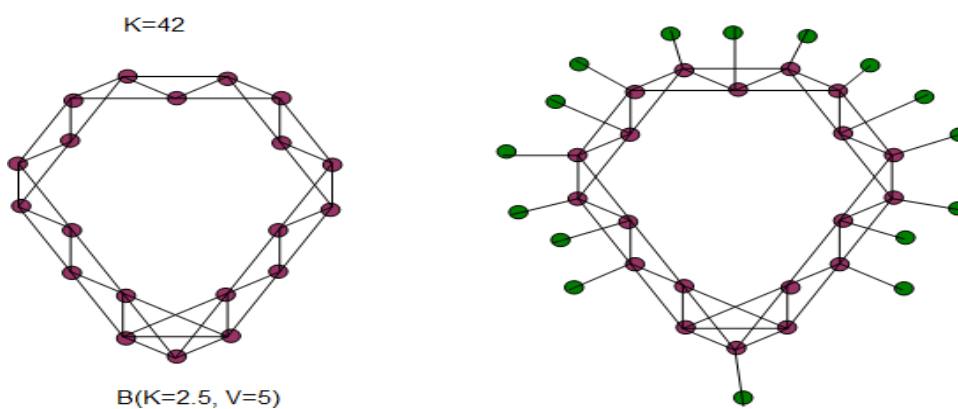


Figure 64. Isomeric graphical structure of $B_{20}H_{16}$

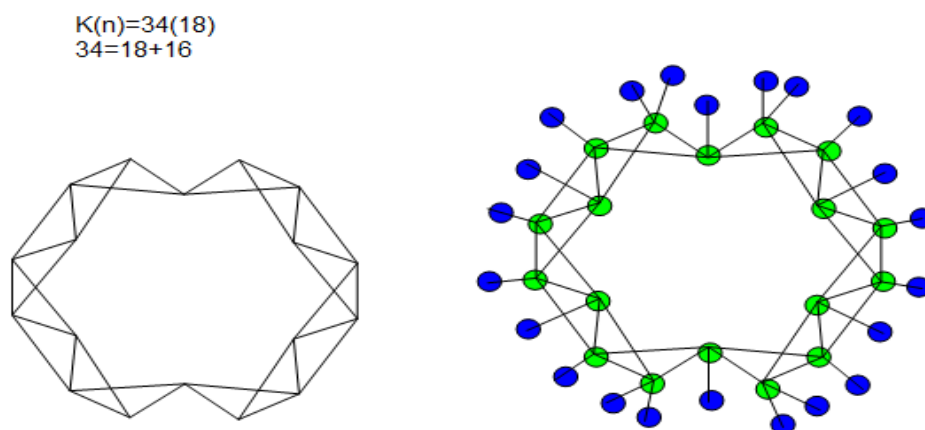


Figure 65. Isomeric graphical structure of $B_{18}H_{22}$

Table 1. Categorization of Borane Clusters into Clan Series

	Cluster	K(n)	S=4n+q	Local name	K*= C ^y +D ^z	y, z	VE0=2z+2	VE=2y+4z+2	VF
1	BH ₃	1(1)	4n+2	closo	C ⁰ +D ¹	0,1	2[1] +2=4	2[0] +4[1] +2=6	1[3] +3=6
2	BH ₄ ⁻	0(1)	4n+4	nido	C ⁻¹ +D ²	-1,2	2[2] +2=6	2[-1] +4[2] +2=8	1[3] +4+1=8
3	B ₂ H ₆	2(2)	4n+4	nido	C ⁻¹ +D ³	-1,3	2[3] +2=8	2[-1] +4[3] +2=12	2[3] +6=12
4	B ₂ H ₈	1(2)	4n+6	arachno	C ⁻² +D ⁴	-2,4	2[4] +2=10	2[-2] +4[4] +2=14	2[3] +8=14
5	B ₃ H ₉	3(3)	4n+6	arachno	C ⁻² +D ⁵	-2,5	2[5] +2=12	2[-2] +4[5] +2=18	3[3] +9=18
6	B ₄ H ₈	6(4)	4n+4	nido	C ⁻¹ +D ⁵	-1,5	2[5] +2=12	2[-1] +4[5] +2=20	4[3] +8=20
7	B ₅ H ₅ ²⁻	9(5)	4n+2	closo	C ⁰ +D ⁵	0,5	2[5] +2=12	2[0] +4[5] +2=22	5[3] +5+2=22
8	B ₄ H ₈	6(4)	4n+4	nido	C ⁻¹ +D ⁵	-1,5	2[5] +2=12	2[-1] +4[5] +2=20	4[3] +8=20
9	B ₃ H ₉	3(3)	4n+6	arachno	C ⁻² +D ⁵	-2,5	2[5] +2=12	2[-2] +4[5] +2=18	3[3] +9=18
10	B ₆ H ₆ ²⁻	11(6)	4n+2	closo	C ⁰ +D ⁶	0,6	2[6] +2=14	2[0] +4[6] +2=26	6[3] +6+2=26
11	B ₅ H ₉	8(5)	4n+4	nido	C ⁻¹ +D ⁶	-1,6	2[6] +2=14	2[-1] +4[6] +2=24	5[3] +9=24
12	B ₄ H ₁₀	5(4)	4n+6	arachno	C ⁻² +D ⁶	-2,6	2[6] +2=14	2[-2] +4[6] +2=22	4[3] +10=22
13	B ₆ H ₁₄	8(6)	4n+8	hypho	C ⁻³ +D ⁹	-3,9	2[9] +2=20	2[-3] +4[9] +2=32	6[3] +14=32
14	B ₇ H ₇ ²⁻	13(7)	4n+2	closo	C ⁰ +D ⁷	0,7	2[7] +2=16	2[0] +4[7] +2=30	7[3] +7+2=30
15	B ₆ H ₁₀	10(6)	4n+4	nido	C ⁻¹ +D ⁷	-1,7	2[7] +2=16	2[-1] +4[7] +2=28	6[3] +10=28
16	B ₅ H ₁₁	7(5)	4n+6	arachno	C ⁻² +D ⁷	-2,7	2[7] +2=16	2[-2] +4[7] +2=26	5[3] +11=26
17	B ₆ H ₁₂	9(6)	4n+6	arachno	C ⁻² +D ⁸	-2,8	2[8] +2=18	2[-2] +4[8] +2=30	6[3] +12=30
18	B ₇ H ₁₁	12(7)	4n+4	nido	C ⁻¹ +D ⁸	-1,8	2[8] +2=18	2[-1] +4[8] +2=32	7[3] +11=32
19	B ₈ H ₈ ²⁻	15(8)	4n+2	closo	C ⁰ +D ⁸	0,8	2[8] +2=18	2[0] +4[8] +2=34	8[3] +8+2=34
20	B ₇ H ₁₁	12(7)	4n+4	nido	C ⁻¹ +D ⁸	-1,8	2[8] +2=18	2[-1] +4[8] +2=32	7[3] +11=32
21	B ₆ H ₁₂	9(6)	4n+6	arachno	C ⁻² +D ⁸	-2,8	2[8] +2=18	2[-2] +4[8] +2=30	6[3] +12=30
22	B ₉ H ₉ ²⁻	17(9)	4n+2	closo	C ⁰ +D ⁹	0,9	2[9] +2=20	2[0] +4[9] +2=38	9[3] +9+2=38
23	B ₈ H ₁₂	14(8)	4n+4	nido	C ⁻¹ +D ⁹	-1,9	2[9] +2=20	2[-1] +4[9] +2=36	8[3] +12=36
24	B ₇ H ₁₃	11(7)	4n+6	arachno	C ⁻² +D ⁹	-2,9	2[9] +2=20	2[-2] +4[9] +2=34	7[3] +13=34
25	B ₆ H ₁₄	8(6)	4n+8	hypho	C ⁻³ +D ⁹	-3, 9	2[9] +2=20	2[-3] +4[9] +2=32	6[3] +14=32
26	B ₉ H ₁₃	16(9)	4n+4	nido	C ⁻¹ +D ¹⁰	-1,10	2[10] +2=22	2[-1] +4[10] +2=40	9[3] +13=40
27	B ₈ H ₁₄	13(8)	4n+6	arachno	C ⁻² +D ¹⁰	-2,10	2[10] +2=22	2[-2] +4[10] +2=38	8[3] +14=38
28	B ₁₀ H ₁₀ ²⁻	19(10)	4n+2	closo	C ⁰ +D ¹⁰	0,10	2[10] +2=22	2[0] +4[10] +2=42	10[3] +10+2=42
29	B ₉ H ₁₃	16(9)	4n+4	nido	C ⁻¹ +D ¹⁰	-1,10	2[10] +2=22	2[-1] +4[10] +2=40	9[3] +13=40
30	B ₈ H ₁₄	13(8)	4n+6	arachno	C ⁻² +D ¹⁰	-2,10	2[10] +2=22	2[-2] +4[10] +2=38	8[3] +14=38
31	B ₇ H ₁₅	10(7)	4n+8	hypho	C ⁻³ +D ¹⁰	-3, 10	2[10] +2=22	2[-3] +4[10] +2=36	7[3] +15=36
32	B ₁₁ H ₁₁ ²⁻	21(11)	4n+2	closo	C ⁰ +D ¹¹	0,11	2[11] +2=24	2[0] +4[11] +2=46	11[3] +11+2=46
33	B ₁₀ H ₁₄	18(10)	4n+4	nido	C ⁻¹ +D ¹¹	-1,11	2[11] +2=24	2[-1] +4[11] +2=44	10[3] +14=44
34	B ₉ H ₁₅	15(9)	4n+6	arachno	C ⁻² +D ¹¹	-2,11	2[11] +2=24	2[-2] +4[11] +2=42	9[3] +15=42
35	B ₈ H ₁₆	12(8)	4n+8	hypho	C ⁻³ +D ¹¹	-3, 11	2[11] +2=24	2[-3] +4[11] +2=40	8[3] +16=40

36	B ₉ H ₁₅	15(9)	4n+6	arachno	C ⁻² +D ¹¹	-2,11	+2=24 2[11] +2=24	+2=40 2[-2]+4[11] +2=42	9[3]+15=42
37	B ₁₀ H ₁₄	18(10)	4n+4	nido	C ⁻¹ +D ¹¹	-1,11	2[11] +2=24	2[-1]+4[11] +2=44	10[3]+14=44
38	B ₁₂ H ₁₂ ²⁻	23(12)	4n+2	closo	C ⁰ +D ¹²	0,12	2[12] +2=26	2[0]+4[12] +2=50	12[3] +12+2=50
39	B ₁₁ H ₁₅	20(11)	4n+4	nido	C ⁻¹ +D ¹²	-1,12	2[12] +2=26	2[-1]+4[12] +2=48	11[3]+15=48
40	B ₁₀ H ₁₆	17(10)	4n+6	arachno	C ⁻² +D ¹²	-2,12	2[12] +2=26	2[-2]+4[12] +2=46	10[3]+16=46
41	B ₉ H ₁₇	14(9)	4n+8	hypso	C ⁻³ +D ¹²	-3,12	2[12] +2=26	2[-3]+4[12] +2=44	9[3]+17=44
42	B ₈ H ₁₈	11(8)	4n+10	klapo	C ⁻⁴ +D ¹²	-4,12	2[12] +2=26	2[-4]+4[12] +2=42	8[3]+18=42
43	B ₁₃ H ₁₃ ²⁻	25(13)	4n+2	closo	C ⁰ +D ¹³	0,13	2[13] +2=28	2[0]+4[13] +2=54	13[3] +13+2=54
44	B ₁₂ H ₁₆	22(12)	4n+4	nido	C ⁻¹ +D ¹³	-1,13	2[13] +2=28	2[-1]+4[13] +2=52	12[3]+16=52
45	B ₁₁ H ₁₇	19(11)	4n+6	arachno	C ⁻² +D ¹³	-2,13	2[13] +2=28	2[-2]+4[13] +2=50	11[3]+17=50
46	B ₁₀ H ₁₈	16(10)	4n+8	hypso	C ⁻³ +D ¹³	-3,13	2[13] +2=28	2[-3]+4[13] +2=48	10[3]+18=48
47	B ₁₄ H ₁₄ ²⁻	27(14)	4n+2	closo	C ⁰ +D ¹⁴	0,14	2[14] +2=30	2[0]+4[14] +2=58	14[3] +14+2=58
48	B ₁₃ H ₁₇	24(13)	4n+4	nido	C ⁻¹ +D ¹⁴	-1,14	2[14] +2=30	2[-1]+4[14] +2=56	13[3]+17=56
49	B ₁₂ H ₁₈	21(12)	4n+6	arachno	C ⁻² +D ¹⁴	-2,14	2[14] +2=30	2[-2]+4[14] +2=54	12[3]+18=54
50	B ₁₁ H ₁₉	18(11)	4n+8	hypso	C ⁻³ +D ¹⁴	-3,14	2[14] +2=30	2[-3]+4[14] +2=52	11[3]+19=52
51	B ₁₅ H ₁₅ ²⁻	29(15)	4n+2	closo	C ⁰ +D ¹⁵	0,15	2[15] +2=32	2[0]+4[15] +2=62	15[3] +15+2=62
52	B ₁₄ H ₁₈	26(14)	4n+4	ndo	C ⁻¹ +D ¹⁵	-1,15	2[15] +2=32	2[-1]+4[15] +2=60	14[3]+18=60
53	B ₁₃ H ₁₉	23(13)	4n+6	arachno	C ⁻² +D ¹⁵	-2,15	2[15] +2=32	2[-2]+4[15] +2=58	13[3]+19=58
54	B ₁₂ H ₂₀	20(12)	4n+8	hypso	C ⁻³ +D ¹⁵	-3,15	2[15] +2=32	2[-3]+4[15] +2=56	12[3]+20=56
55	B ₁₁ H ₂₁	17(11)	4n+10	klapo	C ⁻⁴ +D ¹⁵	-4,15	2[15] +2=32	2[-4]+4[15] +2=54	11[3]+21=54
56	B ₁₀ H ₂₂	14(10)	4n+12		C ⁻⁵ +D ¹⁵	-5,15	2[15] +2=32	2[-5]+4[15] +2=52	10[3]+22=52
57	B ₉ H ₂₃	11(9)	4n+14		C ⁻⁶ +D ¹⁵	-6,15	2[15] +2=32	2[-5]+4[15] +2=50	9[3]+23=50
58	B ₁₄ H ₂₀	25(14)	4n+6	arachno	C ⁻² +D ¹⁶	-2,16	2[16] +2=34	2[-2]+4[16] +2=62	14[3]+20=62
59	B₂₀H₁₆	42(20)	4n-4	3-cap	C³+D¹⁷	3,17	2[17] +2=36	2[3]+4[17] +2=76	20[3]+16=76
60	B ₁₆ H ₂₀	30(16)	4n+4	nido	C ⁻¹ +D ¹⁷	-1,17	2[17] +2=36	2[-1]+4[17] +2=68	16[3]+20=68
61	B ₁₅ H ₂₃	26(15)	4n+8	hypso	C ⁻³ +D ¹⁸	-3,18	2[18] +2=38	2[-3]+4[18] +2=68	15[3]+23=68
62	B₂₀H₂₀	40(20)	4n+0	1-cp	C¹+D¹⁹	1,19	2[19] +2=40	2[1]+4[19] +2=80	20[3]+20=80
63	B ₁₈ H ₂₂	34(18)	4n+4	nido	C ⁻¹ +D ¹⁹	-1,19	2[19] +2=40	2[-1]+4[19] +2=76	18[3]+22=76
64	B ₂₀ H ₂₂	39(20)	4n+2	closo	C ⁰ +D ²⁰	0,20	2[20] +2=42	2[0]+4[20] +2=82	20[3]+22=82
65	B₂₃H₁₉	48(23)	4n-4	3-cap	C³+D²⁰	3,20	2[20] +2=42	2[3]+4[20] +2=88	23[3]+19=88
66	B ₂₀ H ₂₆	37(20)	4n+6	arachno	C ⁻² +D ²²	-2,22	2[22] +2=46	2[-2]+4[22] +2=86	20[3]+26=86

5. Conventional Capping in Borane Clusters

The proper capping based on 4N series approach is very rare in borane clusters unlike the clusters such as those found in golden and transition metal complexes. According to the sample of clusters analyzed in this paper, only 3 were found. These are $B_{20}H_{16}$, and $K^*=C^3+D^{17}$ (tri-capped) is given in Figure 66, $B_{20}H_{20}$, $K^*=C^1+D^{19}$ (mono-capped) Figure 67 and $B_{23}H_{19}$; $K^*=C^3+D^{20}$.

D^{17}

$$48. F=B_{20}H_{16}; K=20[2.5]-8=42, n=20$$

$$K(n)=42(20)$$

$$2[20]-42=-2$$

$$S=4n-4$$

$$K=2n+2$$

$$K_p=C^3C[M17]$$

$$K^*=C^3+D^{17}$$

$$y=3, z=17$$

$$VE_0=2z+2=2[17]+2=36$$

$$VE=VE_0+2n=36+2[20]=76$$

$$VED_z=4z+2=4[17]+2=70$$

$$VE=VED_z+2y=70+2[3]=76$$

$$VE=2y+4z+2=2[3]+4[17]+2=76$$

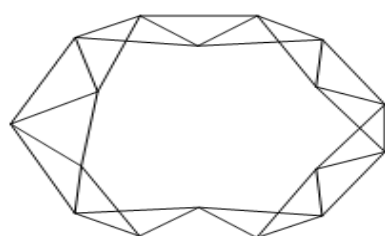
$$VE=8n-2K=8[20]-2[42]=76$$

$$VE=4n-4=4[20]-4=76$$

$$VF=20[3]+16=76$$

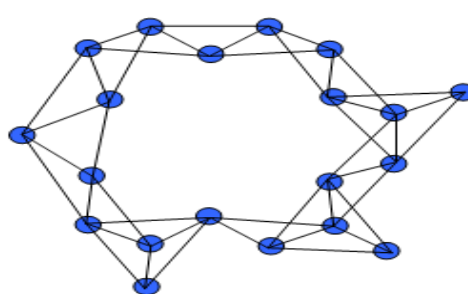
$$VE=VE_0+2y+2z=36+[3]+2[17]=76$$

$$K=2z-1=2[17]-1=33$$



D^{17}

$$K=C^3+D^{17}$$



$$K=33+3[3]=42$$

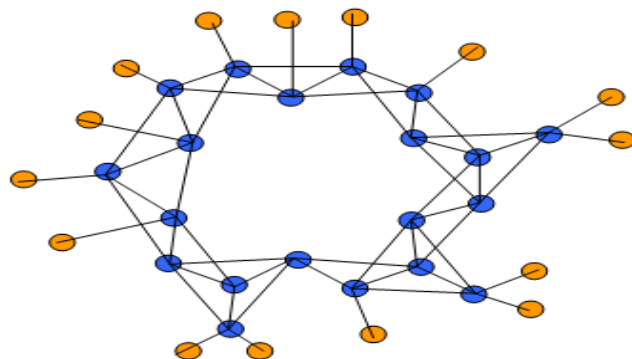


Figure 66. Isomeric graphical structure of $B_{20}H_{16}$

$$47. B_{20}H_{20}: K=20[2.5]-20 [0.5] =40, n=20$$

$$K(n)=40(20)$$

$$2[20]-40=0$$

$$S=4n+0$$

$$K=2n+0$$

$$K_p=C^1C[M19]$$

$$K^*=C^1+D^{19}$$

$$y=1, z=19$$

$$VE_0=2z+2=2 [19] +2=40$$

$$VED_z=4z+2=4 [19] +2=78$$

$$VE=VE_0+2n=40+2 [20] =40+40=80$$

$$VE=VED_z+2y=78+2[1] =80$$

$$VE=2y+4z+2=2[1] +4 [19] +2=80$$

$$VE=8n-2K=8[20]-2 [40] =80$$

$$VE=4n+0=4 [20] +0=80$$

$$VE=VE_0+2y+2z=40+2 [1] + 2[19] =80$$

$$VF=20 [3] +20=80$$

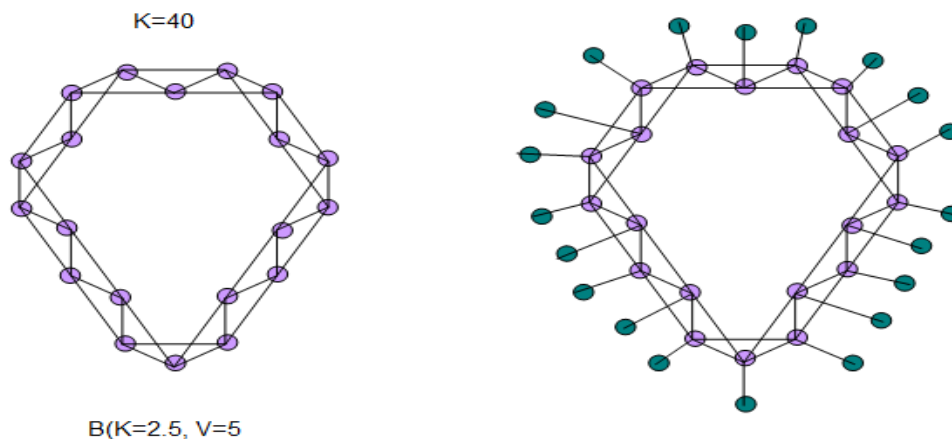


Figure 67. Isomeric graphical structure of $B_{20}H_{20}$

6. Conclusion

The borane clusters have been categorized into clan series. The six newly discovered equations for calculating cluster valence electrons have been demonstrated. The formation of triangles in borane clusters could be associated with the attainment of 5 linkage nodes at borane nodal points and the polyhedral nature of borane clusters. A few rare normal capping borane have been identified. The number of triangles of borane clusters formed using the $4N$ approach for close system are the same as nuclearity index of a cluster. The borane formulas follow a well-organized mathematical sequence.

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