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Numerical Sequence of Borane Series

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ABSTRACT

A table of hydroborane families has been created. The table links boranes of different families(homologous series) and members of the same family based on k number. The table is useful deducing straight away whether a borane(molecular formula) is closo, nido or arachno or something else. The table also indicates that boranes are formed according to natural periodic function (arithmetical progression). The empirical formula utilized is extremely versatile, simple and based on the principle of Nobel gas configuration. It could be used in both simple and complex boranes and carboranes. The closo members which portray characteristic shapes also have characteristic k_1 numbers.

Key words: Numerical sequence, Borane series, closo members.

INTRODUCTION

As a result of the carbon (C) atom to catenate and also form strong bonds with a hydrogen atom, it is able to generate a vast range of families of hydrocarbons. Some of the common families may be given by the formulas

$F_1 = C_nH_{2n+2}$ (alkanes), $F_2 = C_nH_{2n}$ (alkenes), and $F_3 = C_nH_{2n-2}$ (alkynes).

For each of these families, the carbon atom obeys the octet (8) rule which has its base in a noble gas configuration of neon (Ne). On the other hand the boron atom (B) which is next to the carbon atom one valence electron less, mimics the carbon atom to produce boron hydrides (boranes) in an attempt to obey the octet rule. For instance, diborane $B_2H_6 = (BH)_2H_4$ may regarded as attempting to mimic C_2H_4 since (BH) fragment is electronically equivalent to (C) atom. Indeed, their shapes could be viewed as indicated in the sketch of Fig. 1. The two hydrogen atoms indicated by dots in the two bonds, can be considered to donate two electrons into the diboranemolecule so as to enable the boron atoms to satisfy the octet rule. In reality, it should be noted that diborane has two banana bonds of bridging H atoms.

Borane series

Just like hydrocarbons, the known boron

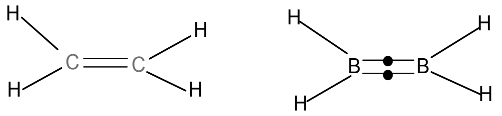

Fig. 1: The relationship between C_2H_{24} and B_2H_6

hydrides have been grouped into families. These families are known as CLOSO, NIDO, ARACHNO and HYPO and the rare one KLADO. These families may be represented by the formulas given below.

$G_0 = B_nH_n$, $G_1 = B_nH_{n+2}$ (CLOSO), $G_2 = B_nH_{n+4}$(NIDO) , $G_3 = B_nH_{n+6}$ (ARACHNO) , $G_4 = B_nH_{n+8}$ (HYPO), $G_5 = B_nH_{n+10}$ (P =KLADO), $G_6 = B_nH_{n+12}$ (Q),$G_7 = B_nH_{n+14}$(R). These series (families) are given in Table 1. Each member of the family has been given a number (k_1 value). The k_1 values are calculated from the empirical formula $k_1 = ½ (E-V)$, where E = sum of octet electrons and V = sum of valence electrons in the cluster. This empirical formula has been discussed in our previous publications[1-2]. What is interesting about the empirical formula is that it predicts a quadruple bond for C_2 diatomic molecule as found from high level theoretical calculation methods[3-4].

Analysis of k_1 values

The k_1 numbers do vary from family to family and also within the members of the same boron family. A movement from one family member to the next family member (horizontally, similar to a period in the periodic table), the k_1 number varies by 1. On the other hand a movement from one member to the next member of the same family(similar to a group in the periodic table), the k_1 number varies by 2. Clearly these are simple arithmetical series. The following examples illustrate this point.

Across families: B_6H_6(12), B_6H_8(11), B_6H_{10}(10), B_6H_{12}(9), B_6H_{14}(8); (simply add or subtract 2H atoms)and across members of the same family: B_5H_7(9), B_6H_8(11), B_7H_9(13), B_8H_{10}(15),

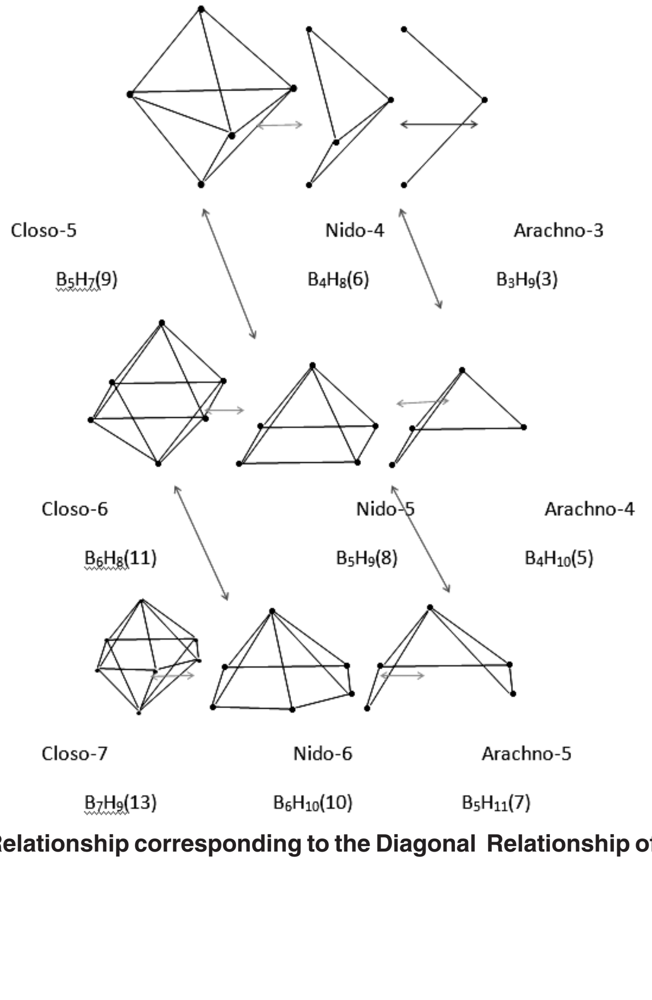

Fig. 2: Geometrical Relationship corresponding to the Diagonal Relationship of k Values of Boranes

Table 1: The k1 Values and the Borane Series

	A	CLOSO	NIDO	ARACHINO	HYPO	P (KLADO)	Q	R
n	B_nH_n	B_nH_{n+2} (k_1)	$B_nH_{n+4}(k_1)$	$B_nH_{n+6}(k_1)$	$B_nH_{n+8}(k_1)$	$B_nH_{n+10}(k_1)$	$B_nH_{n+12}(k_1)$	$B_nH_{n+14}(k_1)$
2	$B_2H_2(4)$	$B_2H_4(3)$	$B_2H_6(2)$	$B_2H_8(1)$	$B_2H_{10}(0)$			
3	$B_3H_3(6)$	$B_3H_5(5)$	$B_3H_7(4)$	$B_3H_9(3)$	$B_3H_{11}(2)$	$B_3H_{13}(1)$	$B_3H_{15}(0)$	
4	$B_4H_4(8)$	$B_4H_6(7)$	$B_4H_8(6)$	$B_4H_{10}(5)$	$B_4H_{12}(4)$	$B_4H_{14}(3)$	$B_4H_{16}(2)$	$B_4H_{18}(1)$
5	$B_5H_5(10)$	$B_5H_7(9)$	$B_5H_9(8)$	$B_5H_{11}(7)$	$B_5H_{13}(6)$	$B_5H_{15}(5)$	$B_5H_{17}(4)$	$B_5H_{19}(3)$
6	$B_6H_6(12)$	$B_6H_8(11)$	$B_6H_{10}(10)$	$B_6H_{12}(9)$	$B_6H_{14}(8)$	$B_6H_{16}(7)$	$B_6H_{18}(6)$	$B_6H_{20}(5)$
7	$B_7H_7(14)$	$B_7H_9(13)$	$B_7H_{11}(12)$	$B_7H_{13}(11)$	$B_7H_{15}(10)$	$B_7H_{17}(9)$	$B_7H_{19}(8)$	$B_7H_{21}(7)$
8	$B_8H_8(16)$	$B_8H_{10}(15)$	$B_8H_{12}(14)$	$B_8H_{14}(13)$	$B_8H_{16}(12)$	$B_8H_{18}(11)$	$B_8H_{20}(10)$	$B_8H_{22}(9)$
9	$B_9H_9(18)$	$B_9H_{11}(17)$	$B_9H_{13}(16)$	$B_9H_{15}(15)$	$B_9H_{17}(14)$	$B_9H_{19}(13)$	$B_9H_{21}(12)$	$B_9H_{23}(11)$
10	$B_{10}H_{10}(20)$	$B_{10}H_{12}(19)$	$B_{10}H_{14}(18)$	$B_{10}H_{16}(17)$	$B_{10}H_{18}(16)$	$B_{10}H_{20}(15)$	$B_{10}H_{22}(14)$	$B_{10}H_{24}(13)$
11	$B_{11}H_{11}(22)$	$B_{11}H_{13}(21)$	$B_{11}H_{15}(20)$	$B_{11}H_{17}(19)$	$B_{11}H_{19}(18)$	$B_{11}H_{21}(17)$	$B_{11}H_{23}(16)$	$B_{11}H_{25}(15)$
12	$B_{12}H_{12}(24)$	$B_{12}H_{14}(23)$	$B_{12}H_{16}(22)$	$B_{12}H_{18}(21)$	$B_{12}H_{20}(20)$	$B_{12}H_{22}(19)$	$B_{12}H_{24}(18)$	$B_{12}H_{26}(17)$
13	$B_{13}H_{13}(26)$	$B_{13}H_{15}(25)$	$B_{13}H_{17}(24)$	$B_{13}H_{19}(23)$	$B_{13}H_{21}(22)$	$B_{13}H_{23}(21)$	$B_{13}H_{25}(20)$	$B_{13}H_{27}(19)$
14	$B_{14}H_{14}(28)$	$B_{14}H_{16}(27)$	$B_{14}H_{18}(26)$	$B_{14}H_{20}(25)$	$B_{14}H_{22}(24)$	$B_{14}H_{24}(23)$	$B_{14}H_{26}(22)$	$B_{14}H_{28}(21)$
15	$B_{15}H_{15}(30)$	$B_{15}H_{17}(29)$	$B_{15}H_{19}(28)$	$B_{15}H_{21}(27)$	$B_{15}H_{23}(26)$	$B_{15}H_{25}(25)$	$B_{15}H_{27}(24)$	$B_{15}H_{29}(23)$
16	$B_{16}H_{16}(32)$	$B_{16}H_{18}(31)$	$B_{16}H_{20}(30)$	$B_{16}H_{22}(29)$	$B_{16}H_{24}(28)$	$B_{16}H_{26}(27)$	$B_{16}H_{28}(26)$	$B_{16}H_{30}(25)$
17	$B_{17}H_{17}(34)$	$B_{17}H_{19}(33)$	$B_{17}H_{21}(32)$	$B_{17}H_{23}(31)$	$B_{17}H_{25}(30)$	$B_{17}H_{27}(29)$	$B_{17}H_{29}(28)$	$B_{17}H_{31}(27)$
18	$B_{18}H_{18}(36)$	$B_{18}H_{20}(35)$	$B_{18}H_{22}(34)$	$B_{18}H_{24}(33)$	$B_{18}H_{26}(32)$	$B_{18}H_{28}(31)$	$B_{18}H_{30}(30)$	$B_{18}H_{32}(29)$
19	$B_{19}H_{19}(38)$	$B_{19}H_{21}(37)$	$B_{19}H_{23}(36)$	$B_{19}H_{25}(35)$	$B_{19}H_{27}(34)$	$B_{19}H_{29}(33)$	$B_{19}H_{31}(32)$	$B_{19}H_{33}(31)$
20	$B_{20}H_{20}(40)$	$B_{20}H_{22}(39)$	$B_{20}H_{24}(38)$	$B_{20}H_{26}(37)$	$B_{20}H_{28}(36)$	$B_{20}H_{30}(35)$	$B_{20}H_{32}(34)$	$B_{20}H_{34}(33)$
21	$B_{21}H_{21}(42)$	$B_{21}H_{23}(41)$	$B_{21}H_{25}(40)$	$B_{21}H_{27}(39)$	$B_{21}H_{29}(38)$	$B_{21}H_{31}(37)$	$B_{21}H_{33}(36)$	$B_{21}H_{35}(35)$
22	$B_{22}H_{22}(44)$	$B_{22}H_{24}(43)$	$B_{22}H_{26}(42)$	$B_{22}H_{28}(41)$	$B_{22}H_{30}(40)$	$B_{22}H_{32}(39)$	$B_{22}H_{34}(38)$	$B_{22}H_{36}(37)$
24	$B_{23}H_{23}(46)$	$B_{23}H_{25}(45)$	$B_{23}H_{27}(44)$	$B_{23}H_{29}(43)$	$B_{23}H_{31}(42)$	$B_{23}H_{33}(41)$	$B_{23}H_{35}(40)$	$B_{23}H_{37}(39)$
24	$B_{24}H_{24}(48)$	$B_{24}H_{26}(47)$	$B_{24}H_{28}(46)$	$B_{24}H_{30}(45)$	$B_{24}H_{32}(44)$	$B_{24}H_{34}(43)$	$B_{24}H_{36}(42)$	$B_{24}H_{38}(41)$
25	$B_{25}H_{25}(50)$	$B_{25}H_{27}(49)$	$B_{25}H_{29}(48)$	$B_{25}H_{31}(47)$	$B_{25}H_{33}(46)$	$B_{25}H_{35}(45)$	$B_{25}H_{37}(44)$	$B_{25}H_{39}(43)$
26	$B_{26}H_{26}(52)$	$B_{26}H_{28}(51)$	$B_{26}H_{30}(50)$	$B_{26}H_{32}(49)$	$B_{26}H_{34}(48)$	$B_{26}H_{36}(47)$	$B_{26}H_{38}(46)$	$B_{26}H_{40}(45)$
27	$B_{27}H_{27}(54)$	$B_{27}H_{29}(53)$	$B_{27}H_{31}(52)$	$B_{27}H_{33}(51)$	$B_{27}H_{35}(50)$	$B_{27}H_{37}(49)$	$B_{27}H_{39}(48)$	$B_{27}H_{41}(47)$
28	$B_{28}H_{28}(56)$	$B_{28}H_{30}(55)$	$B_{28}H_{32}(54)$	$B_{28}H_{34}(53)$	$B_{28}H_{36}(52)$	$B_{28}H_{38}(51)$	$B_{28}H_{40}(50)$	$B_{28}H_{42}(49)$
29	$B_{29}H_{29}(58)$	$B_{29}H_{31}(57)$	$B_{29}H_{33}(56)$	$B_{29}H_{35}(55)$	$B_{29}H_{37}(54)$	$B_{29}H_{39}(53)$	$B_{29}H_{41}(52)$	$B_{29}H_{43}(51)$
30	$B_{30}H_{30}(60)$	$B_{30}H_{32}(59)$	$B_{30}H_{34}(58)$	$B_{30}H_{36}(57)$	$B_{30}H_{38}(56)$	$B_{30}H_{40}(55)$	$B_{30}H_{42}(54)$	$B_{30}H_{44}(53)$

Table 2: Diagonal Relationship of k Values ofBoranes for n =2 to 12

Geometry of Closo	Formula of Closo		Possible Closo Neutral Formula	NIDO	Arachino
		n	B_nH_{n+2} (k_1)	B_nH_{n+4}(k_1)	B_nH_{n+6}(k_1)
		2	B_2H_4(3)	B_2H_6(2)	B_2H_8(1)
		3	B_3H_5(5)	B_3H_7(4)	B_3H_9(3)
Tetrahedral, T_d	$B_4H_4^{2-}$	4	B_4H_6(7)	B_4H_8(6)	B_4H_{10}(5)
Trigonalbipyramid, D_{3h}	$B_5H_5^{2-}$	5	B_5H_7(9)	B_5H_9(8)	B_5H_{11}(7)
Octahedral, O_h	$B_6H_6^{2-}$	6	B_6H_8(11)	B_6H_{10}(10)	B_6H_{12}(9)
Pentagonal bipyramid, D_{5h}	$B_7H_7^{2-}$	7	B_7H_9(13)	B_7H_{11}(12)	B_7H_{13}(11)
Dodecahedron, D_{2d}	$B_8H_8^{2-}$	8	B_8H_{10}(15)	B_8H_{12}(14)	B_8H_{14}(13)
TricappedTrigonalPriam, D_{3h}	$B_9H_9^{2-}$	9	B_9H_{11}(17)	B_9H_{13}(16)	B_9H_{15}(15)
Bicapped Square Antiprism, D_{4d}	$B_{10}H_{10}^{2-}$	10	$B_{10}H_{12}$(19)	$B_{10}H_{14}$(18)	$B_{10}H_{16}$(17)
Octadecahedron, C_{2v}	$B_{11}H_{11}^{2-}$	11	$B_{11}H_{13}$(21)	$B_{11}H_{15}$(20)	$B_{11}H_{17}$(19)
Icosahedron, I_h	$B_{12}H_{12}^{2-}$	12	$B_{12}H_{14}$(23)	$B_{12}H_{16}$(22)	$B_{12}H_{18}$(21)

Table 3: Geometrical Relationship corresponding to the Diagonal Relationship of k Values of Boranes

n	CLOSO	NIDO	ARACHNO
	B_nH_{n+2}(k_1)	B_{n+4}(k_1)	B_{n+6}(k_1)
	n	n-1	n-2
3	B_3H_5(5)	B_2H_6(2)	
4	B_4H_6(7)	B_3H_7(4)	B_2H_8(1)
5	B_5H_7(9)	B_4H_8(6)	B_3H_9(3)
6	B_6H_8(11)	B_5H_9(8)	B_4H_{10}(5)
7	B_7H_9(13)	B_6H_{10}(10)	B_5H_{11}(7)
8	B_8H_{10}(15)	B_7H_{11}(12)	B_6H_{12}(9)
9	B_9H_{11}(17)	B_8H_{12}(14)	B_7H_{13}(11)
10	$B_{10}H_{12}$(19)	B_9H_{13}(16)	B_8H_{14}(13)
11	$B_{11}H_{13}$(21)	$B_{10}H_{14}$(18)	B_9H_{15}(15)
12	$B_{12}H_{14}$(23)	$B_{11}H_{15}$(20)	$B_{10}H_{16}$(17)

B_9H_{11}(17), $B_{10}H_{12}$(19), $B_{11}H_{13}$(21), $B_{12}H_{14}$(23)(simply add or subtract BH fragment). A large number of hypothetical neutral boranes expected from the formulas have never been synthesized. For instance, the neutral members of the closo family, B_5H_7, B_6H_8, B_7H_9, B_8H_{10}, B_9H_{11}, $B_{10}H_{12}$, $B_{11}H_{13}$, and $B_{12}H_{14}$ have not been observed instead $B_5H_5^{\text{Ë\#2}-}$, $B_6H_6^{\text{Ë\#2}-}$, $B_7H_7^{\text{Ë\#2}-}$, $B_8H_8^{\text{Ë\#2}-}$, $B_9H_9^{\text{Ë\#2}-}$, $B_{10}H_{10}^{\text{Ë\#2}-}$, $B_{11}H_{11}^{\text{Ë\#2}-}$, and $B_{12}H_{12}^{\text{Ë\#2}-}$, are well known. In Table 1, it hasbeen found easier to explain the series by assuming that all boranes are neutral. For instance to test to which family a hydroborane belongs, $B_2H_7^{\text{Ë\#}-}$ is regarded as B_2H_8 and $B_5H_8^{\text{Ë\#}-}$ as B_5H_9. A collection sample of boranes have been classified based on Table 1 and these are presented in Table 5.

Table 4: Geometrical Relationship in Fig. 1 expressed in k_1 values

	Starting Cluster	Closo	NIDO	Arachno
	-B + H			
+ B H	B_4H_6 ($B_4H_4^{2-}$)	7	4	1
	B_5H_7 ($B_5H_5^{2-}$)	9	6	3
	B_6H_8($B_6H_6^{2-}$)	11	8	5
	B_7H_9($B_7H_7^{2-}$)	13	10	7
	B_8H_{10}($B_8H_8^{2-}$)	15	12	9
	B_9H_{11}($B_9H_9^{2-}$)	17	14	11
	$B_{10}H_{12}$($B_{10}H_{10}^{2-}$)	19	16	13
	$B_{11}H_{13}$($B_{11}H_{11}^{2-}$)	21	18	15
	$B_{12}H_{14}$($B_{12}H_{12}^{2-}$)	23	20	17

Table 5: Selected Examples of Boranes for Classification Using Table 1

B_n	Examples	Proposed Classification
1		
2	B_2H_6, B_2H_8	NAR
3	B_3H_9	AR
4	B_4H_8,	N
	B_4H_{10}	AR
5	B_5H_7, B_5H_9,	CN
	B_5H_{11}	AR
	B_5H_{13}	H
6	B_6H_8,	C
	$B_6H_{10}B_6H_{12}$	NAR
7	$B_7H_9B_7H_{13}$	C
8	B_8H_{10},	C
	B_8H_{12},	N
	B_8H_{14},	AR
	B_8H_{16}	H
	B_8H_{18}	P
9	B_9H_{11}	C
	B_9H_{13},	N
	B_9H_{15}	AR
10	$B_{10}H_{12}$,	C
	$B_{10}H_{14}$,	N
	$B_{10}H_{16}$,	AR
	$B_{10}H_{18}$	H

Diagonal relationship within the families

The diagonal relationship within boranec families can readily be discerned from Table 1. The examples include B_5H_7(9)'! B_4H_8(6)'! B_3H_9(3); and B_6H_8(11)'! B_5H_9(8)'! B_4H_{10}(5). This diagonal relationship also presented horizontally in Table 3, is cited widely in form of shapes[5] and is partially presented in Fig. 1. The k_1 numbers vary by 3 units. The diagonal relationship within boron families when set up horizontally, another diagonal relationship is detected. The variations are given in Table 4. This relationship links up boranes with the same number of B atoms but different number of hydrogen atoms from different families. For instance, B_5H_7(9) (CLOSO)'! B_5H_9(8)(NIDO)'! B_5H_{11}(7)(ARACHNO). The $k_1$values vary by 1 and therefore the shapes differ.It has also been found from theoretical studies by Yao and Hoffman[6] that the boranes B_3H_9 , B_4H_{12} and B_6H_{18} have some stability with B_6H_{18} being the most stable. These boranes belong to the families, ARACHNO, HYPO, and P (see Table 1) respectively. Furthermore, theoretical calculations[7] indicate that the boranesB_4H_2, $B_4H_{24,}$ B_4H_6, B_4H_8 and B_4H_{10}(belong to the families B,C, N, AR in the Table 1) are more stable than B_4H, B_4H_3, B_4H_5, B_4H_7, and B_4H_9 which do not belong to any of the families.

Table 1: Extended left wise

	G	F	E	D	C_0
n	B_nH_{n-10}	B_nH_{n-8}	B_nH_{n-6}	B_nH_{n-4}	B_nH_{n-2}
1	0	0	0	0	0
2	0	0	0	0	B_2
3	0	0	0	0	B_3H
4	0	0	0	B_4	B_4H_2
5	0	0	0	B_5H	B_5H_3
6	0	0	B_6	B_6H_2	B_6H_4
7	0	0	B_7H	B_7H_3	B_7H_5
8	0	B_8	B_8H_2	B_8H_4	B_8H_6
9	0	B_9H	B_9H_3	B_9H_5	B_9H_7
10	B_{10}	$B_{10}H_2$	$B_{10}H_4$	$B_{10}H_6$	$B_{10}H_8$
11	$B_{11}H$	$B_{11}H_3$	$B_{11}H_5$	$B_{11}H_7$	$B_{11}H_9$
12	$B_{12}H_2$	$B_{12}H_4$	$B_{12}H_6$	$B_{12}H_8$	$B_{12}H_{10}$
13	$B_{13}H_3$	$B_{13}H_5$	$B_{13}H_7$	$B_{13}H_9$	$B_{13}H_{11}$
14	$B_{14}H_4$	$B_{14}H_6$	$B_{14}H_8$	$B_{14}H_{10}$	$B_{14}H_{12}$
15	$B_{15}H_5$	$B_{15}H_7$	$B_{15}H_9$	$B_{15}H_{11}$	$B_{15}H_{13}$
16	$B_{16}H_6$	$B_{16}H_8$	$B_{16}H_{10}$	$B_{16}H_{12}$	$B_{16}H_{14}$
17	$B_{17}H_7$	$B_{17}H_9$	$B_{17}H_{11}$	$B_{17}H_{13}$	$B_{17}H_{15}$
18	$B_{18}H_8$	$B_{18}H_{10}$	$B_{18}H_{12}$	$B_{18}H_{14}$	$B_{18}H_{16}$
19	$B_{19}H_9$	$B_{19}H_{11}$	$B_{19}H_{13}$	$B_{19}H_{15}$	$B_{19}H_{17}$
20	$B_{20}H_{10}$	$B_{20}H_{12}$	$B_{20}H_{14}$	$B_{20}H_{16}$	$B_{20}H_{18}$

Table 1 has been extended on the left to cover the boron families headed by symbols C_0, D, E, and G. The whole Table 1 covers the series B_nH_{n-10} to $B_nH_{n+14.}$

CONCLUSION

Borane series tend to occur in families just like hydrocarbons. The driving force for cluster formation is probably due to boranes attempting to obey the octet rule. A given borane that obeys the octet rule may be classified to belong to a particle family using the table. Both the known boranes and the theoretically established as being stable appear to fit into one of the families. Just as the elements of the periodic table follow a simple arithmetical progression, the boranes across the row horizontally (families- similar to the period in the periodic table)) and vertically(within the family members- similar to a group within the periodic table) as well as diagonally (similar to the diagonal relationship of elements in the periodic table) follow simple arithmetical progression. The k_1 values are useful in organizing the boron families and their members.

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