

Perfectly Concentric Planar π -Aromatic $B_{18}H_3^-$, $B_{18}H_4$, $B_{18}H_5^+$, and $B_{18}H_6^{2+}$: Inorganic Analogues of [10]Annulene

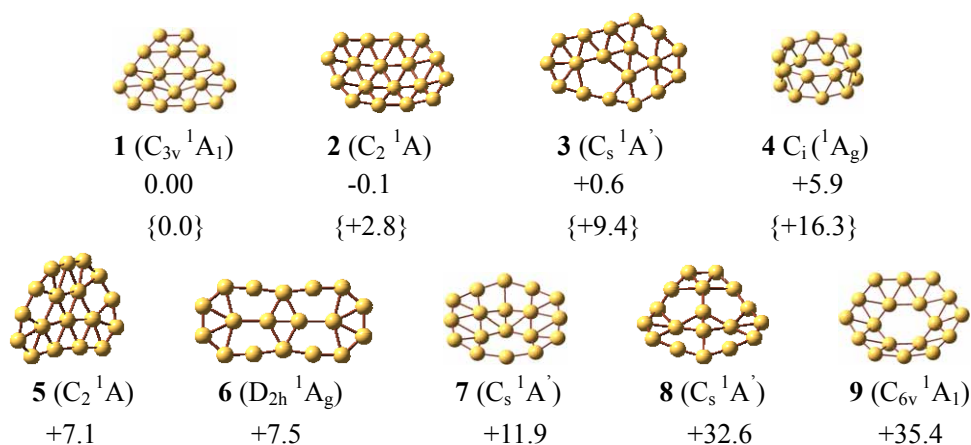
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Institute of Materials Science and Department of Chemistry, Xinzhou Teachers' University, Xinzhou
034000, Shanxi, People's Republic of China. E-mail: lisidian@yahoo.com*

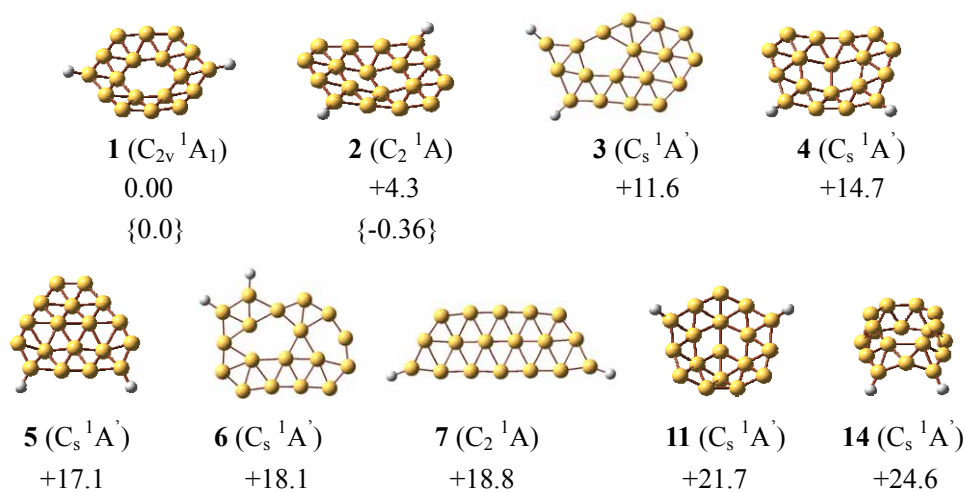
Supplementary Information

Fig.1S Low-lying isomers obtained for concerned borannulenes and their cations and anions with relative energies indicated in kcal/mol at B3LYP/6-311G(d,p) and {CCSD(T)//B3LYP}

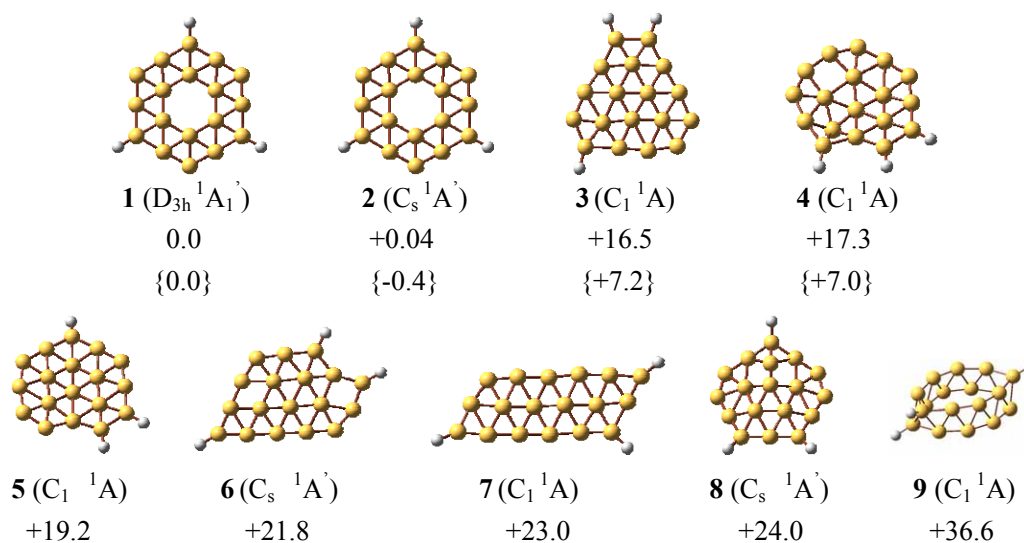
1. B₁₈ neutral



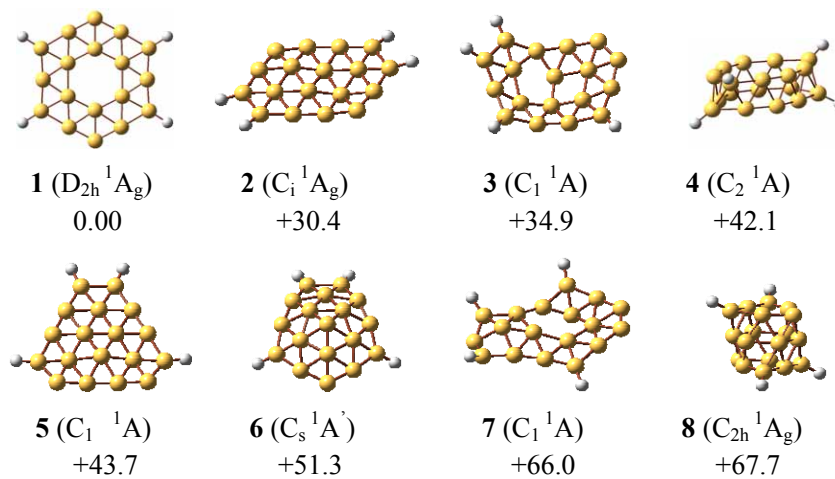
2. B₁₈H₂ neutral



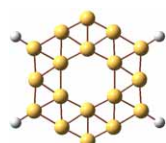
3. B₁₈H₃⁻ anion



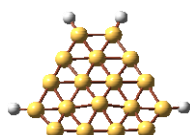
4. B₁₈H₄ neutral



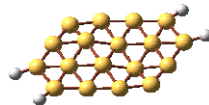
5. $B_{18}H_4^-$ anion



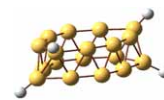
1 ($D_{2h}^2 B_{2g}$)
0.0



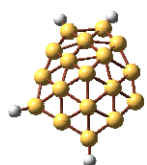
2 ($C_1^2 A$)
+19.9



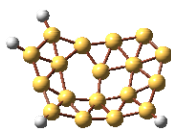
3 ($C_i^2 A_g$)
+24.1



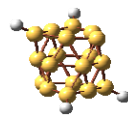
4 ($C_2^2 A$)
+30.8



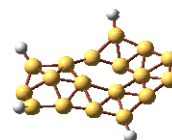
5 ($C_1^2 A$)
+33.7



6 ($C_1^2 A$)
+34.8

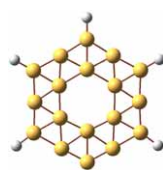


7 ($C_{2h}^2 A$)
+56.7

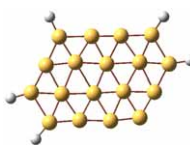


8 ($C_1^2 A$)
+61.5

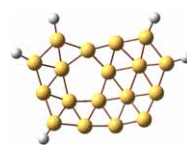
6. $B_{18}H_5^+$ cation



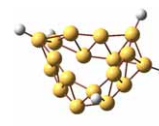
1 ($C_{2v}^1 A_1$)
0.0



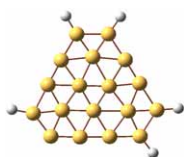
2 ($C_1^1 A$)
+26.7



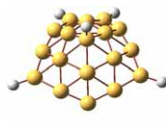
3 ($C_1^1 A$)
+35.0



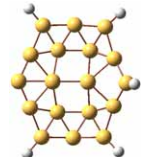
4 ($C_1^1 A$)
+37.1



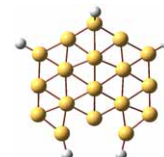
5 ($C_1^1 A$)
+49.0



6 ($C_s^1 A'$)
+53.0

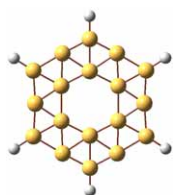


7 ($C_s^1 A'$)
+56.3

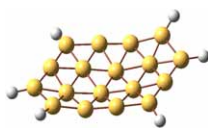


8 ($C_s^1 A'$)
+56.4

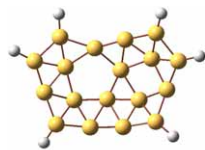
7. $B_{18}H_6^{2+}$ dication



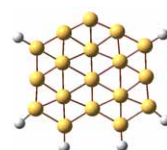
1 ($D_{6h}^1 A_g$)
0.0



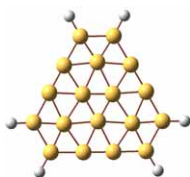
2 ($C_{2v}^1 A$)
+51.3



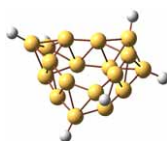
3 ($C_{1v}^1 A$)
+53.1



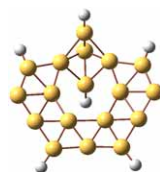
4 ($C_s^1 A'$)
+57.0



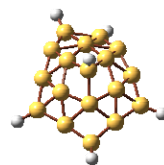
5 ($D_{3h}^3 A_1'$)
+66.0



6 ($C_{2v}^1 A$)
+80.6

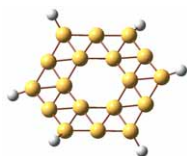


7 ($C_s^1 A'$)
+88.3

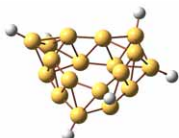


8 ($C_{1v}^1 A$)
+95.0

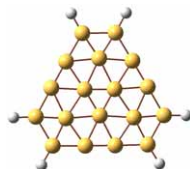
8. $B_{18}H_6$ neutral



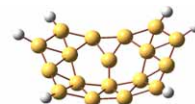
1 ($D_{3d}^1 A_g$)
0.0
{0.0}



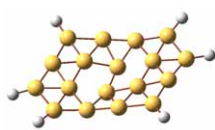
2 ($D_3^1 A_1$)
+0.6
{-29.5}



3 ($D_{3h}^1 A_1'$)
+11.4
{+3.2}



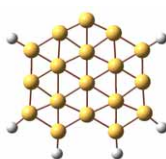
4 ($C_s^1 A'$)
+18.3
{+14.1}



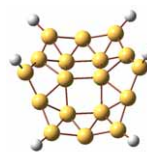
5 ($C_{2v}^1 A$)
+19.1



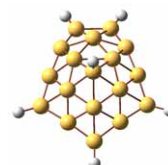
6 ($D_{6h}^1 A_{1g}$)
+19.3



7 ($C_{2v}^1 A_1$)
+30.1



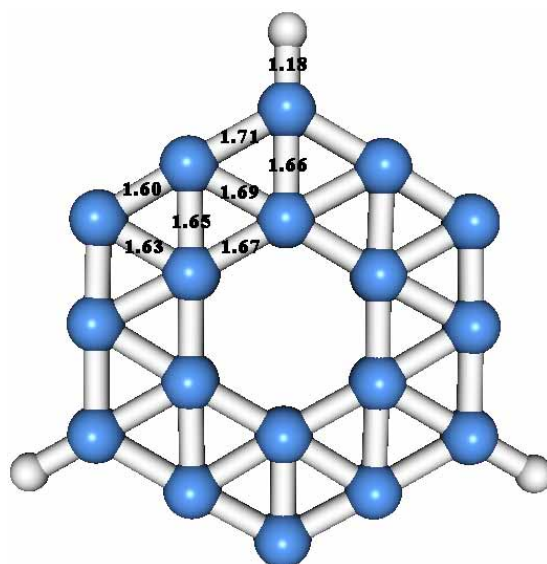
8 ($C_{2v}^1 A_1$)
+35.9



9 ($C_s^1 A'$)
+36.2

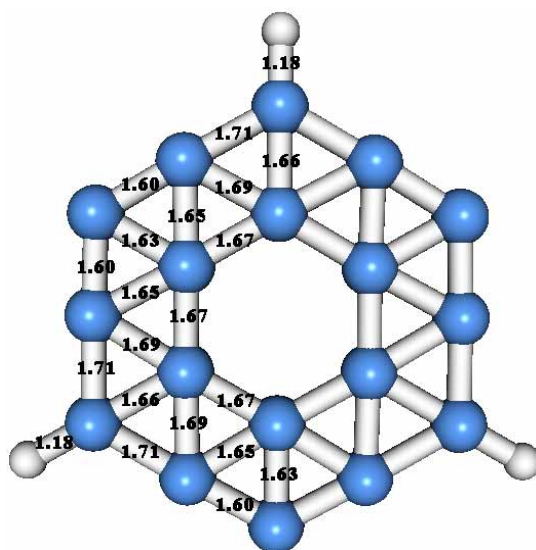
Fig.2S Optimized bond lengths and Cartesian coordinates (x, y, z) in Å
for D_{3h} $B_{18}H_3^-$ (**6**) (a), C_s $B_{18}H_3^-$ (**15**) (b), D_{2h} $B_{18}H_4$ (**8**) (c), C_{2v} $B_{18}H_5^+$ (**10**)
(d), and D_{6h} $B_{18}H_6^{2+}$ (**12**) (e) at B3LYP/6-311(d,p)

(a). D_{3h} $B_{18}H_3^-$



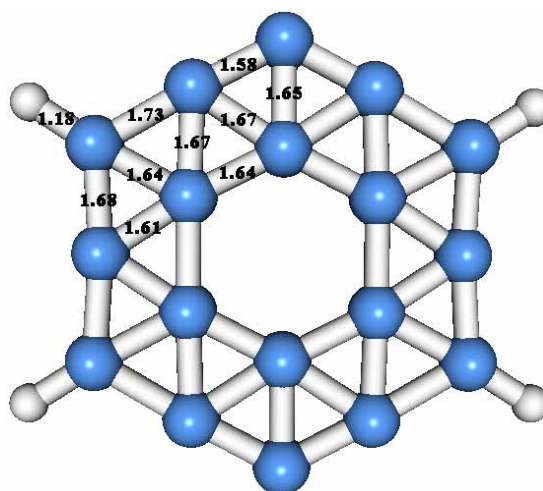
Atomic Number	X	Y	Z
5	2.849859	-1.645367	0.000000
5	0.000000	1.661666	0.000000
5	-1.439045	-0.830833	0.000000
5	1.439045	-0.830833	0.000000
5	1.446921	0.835380	0.000000
5	0.000000	-1.670760	0.000000
5	1.483335	-2.479969	0.000000
5	0.000000	-3.329809	0.000000
5	-1.446921	0.835380	0.000000
5	2.883700	1.664905	0.000000
5	2.889384	-0.044621	0.000000
5	0.000000	3.290734	0.000000
5	1.406049	2.524591	0.000000
5	-1.483335	-2.479969	0.000000
5	-2.849859	-1.645367	0.000000
5	-2.883700	1.664905	0.000000
5	-1.406049	2.524591	0.000000
5	-2.889384	-0.044621	0.000000
1	3.908170	2.256383	0.000000
1	-3.908170	2.256383	0.000000
1	0.000000	-4.512767	0.000000

(b). $C_s B_{18}H_3^-$



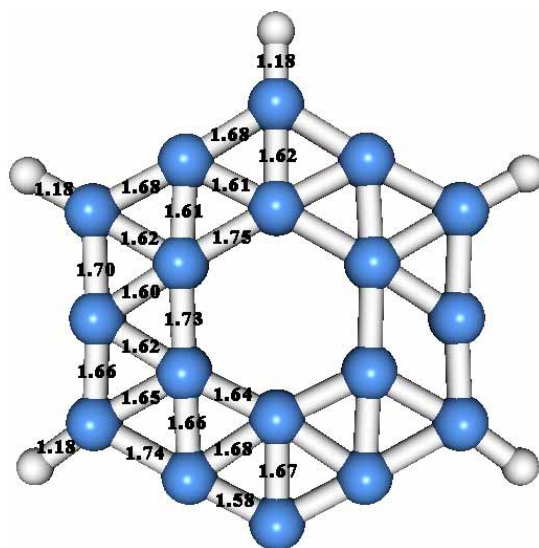
Atomic Number	X	Y	Z
5	1.642246	-0.083572	2.842072
5	-1.659108	-0.105255	0.000000
5	0.827271	0.112662	-1.442326
5	0.827271	0.112662	1.442326
5	-0.833315	-0.021029	1.445457
5	1.669348	0.157897	0.000000
5	2.474950	0.012028	1.479902
5	3.322459	-0.010958	0.000000
5	-0.833315	-0.021029	-1.445457
5	-1.663039	-0.028537	2.882733
5	0.045810	-0.067540	2.887402
5	-3.279700	0.087593	0.000000
5	-2.519456	0.029595	1.404963
5	2.474950	0.012028	-1.479902
5	1.642246	-0.083572	-2.842072
5	-1.663039	-0.028537	-2.882733
5	-2.519456	0.029595	-1.404963
5	0.045810	-0.067540	-2.887402
1	-2.255773	-0.038342	-3.906448
1	-2.255773	-0.038342	3.906448
1	4.501878	-0.105764	0.000000

(c). D_{2h} $B_{18}H_4$



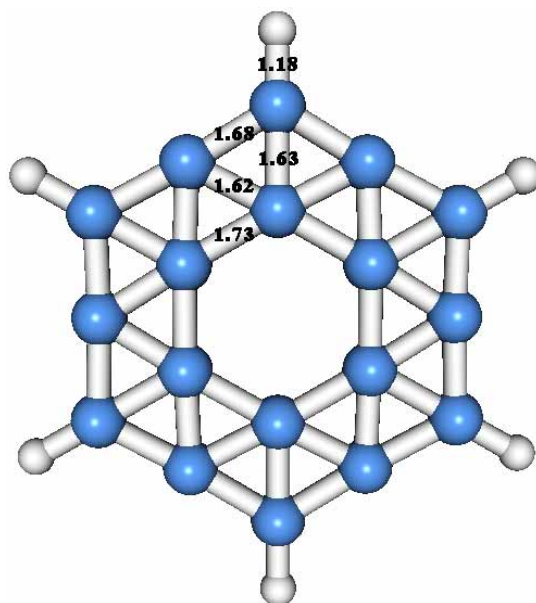
Atomic Number	X	Y	Z
5	0.000000	2.893649	1.677953
5	0.000000	0.000000	-1.641631
5	0.000000	-1.459833	0.890745
5	0.000000	1.459833	0.890745
5	0.000000	1.459833	-0.890745
5	0.000000	0.000000	1.641631
5	0.000000	1.398446	2.556769
5	0.000000	0.000000	3.293392
5	0.000000	-1.459833	-0.890745
5	0.000000	2.893649	-1.677953
5	0.000000	2.798093	0.000000
5	0.000000	0.000000	-3.293392
5	0.000000	1.398446	-2.556769
5	0.000000	-1.398446	2.556769
5	0.000000	-2.893649	1.677953
5	0.000000	-2.893649	-1.677953
5	0.000000	-1.398446	-2.556769
5	0.000000	-2.798093	0.000000
1	0.000000	3.885759	2.314344
1	0.000000	-3.885759	-2.314344
1	0.000000	-3.885759	2.314344
1	0.000000	3.885759	-2.314344

(d). C_{2v} $B_{18}H_5^+$



Atomic Number	X	Y	Z
5	0.000000	2.918520	1.635312
5	0.000000	0.000000	-1.642004
5	0.000000	-1.518640	0.811666
5	0.000000	1.518640	0.811666
5	0.000000	1.472409	-0.922415
5	0.000000	0.000000	1.687525
5	0.000000	1.431287	2.420295
5	0.000000	0.000000	3.305790
5	0.000000	-1.472409	-0.922415
5	0.000000	2.910763	-1.726553
5	0.000000	2.852469	-0.065379
5	0.000000	0.000000	-3.312522
5	0.000000	1.393389	-2.577672
5	0.000000	-1.431287	2.420295
5	0.000000	-2.918520	1.635312
5	0.000000	-2.910763	-1.726553
5	0.000000	-1.393389	-2.577672
5	0.000000	-2.852469	-0.065379
1	0.000000	3.860367	-2.423904
1	0.000000	3.947925	2.208393
1	0.000000	-3.860367	-2.423904
1	0.000000	-3.947925	2.208393
1	0.000000	0.000000	4.484533

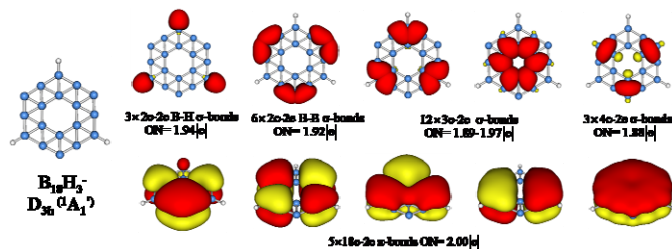
(e). D_{6h} $B_{18}H_6^{2+}$



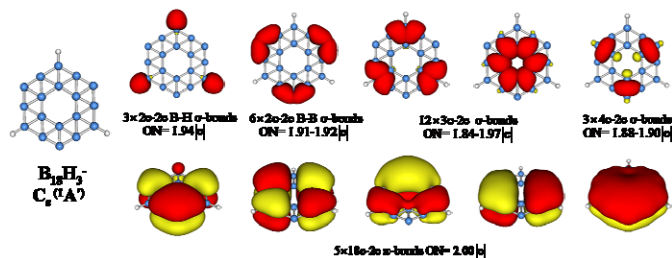
Atomic Number	X	Y	Z
5	2.911626	-1.681028	0.000000
5	0.000000	1.731901	0.000000
5	-1.499870	-0.865950	0.000000
5	1.499870	-0.865950	0.000000
5	1.499870	0.865950	0.000000
5	0.000000	-1.731901	0.000000
5	1.431709	-2.479793	0.000000
5	0.000000	-3.362056	0.000000
5	-1.499870	0.865950	0.000000
5	2.911626	1.681028	0.000000
5	2.863418	0.000000	0.000000
5	0.000000	3.362056	0.000000
5	1.431709	2.479793	0.000000
5	-1.431709	-2.479793	0.000000
5	-2.911626	-1.681028	0.000000
5	-2.911626	1.681028	0.000000
5	-1.431709	2.479793	0.000000
5	-2.863418	0.000000	0.000000
1	3.935010	-2.271879	0.000000
1	-3.935010	2.271879	0.000000
1	-3.935010	-2.271879	0.000000
1	3.935010	2.271879	0.000000
1	0.000000	4.543758	0.000000
1	0.000000	-4.543758	0.000000

Fig.3S AdNDP bonding patterns obtained for D_{3h} $B_{18}H_3^-$ (**6**), D_{2h} $B_{18}H_4$ (**8**), C_{2v} $B_{18}H_5^+$ (**c**), and D_{6h} $B_{18}H_6^{2+}$ (**12**) (d) at B3LYP/6-31G.

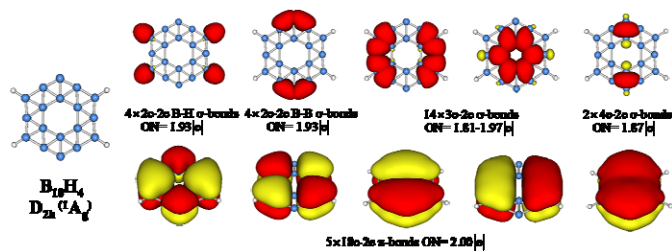
(a). D_{3h} $B_{18}H_3^-$



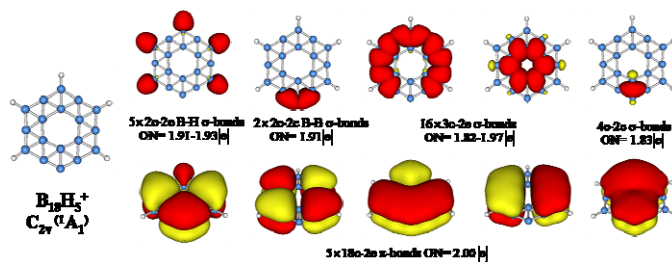
(b). C_s $B_{18}H_3^-$



(c). D_{2h} $B_{18}H_4$



(d). C_{2v} $B_{18}H_5^+$



(e). D_{6h} $B_{18}H_6^{2+}$

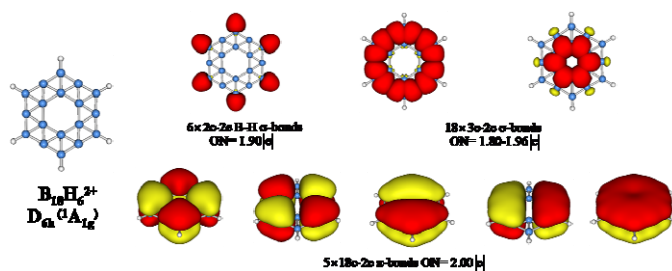


Fig.4S Simulated UV spectrum of D_{2h} $B_{18}H_4$ at TD-B3LYP

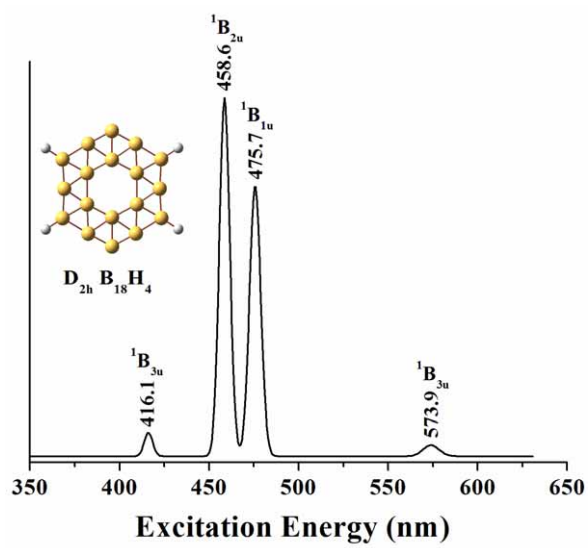
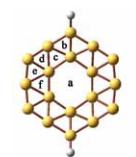
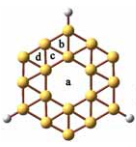
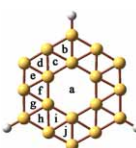
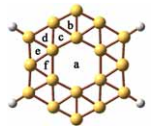

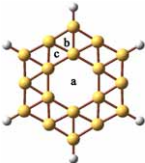


Table 1S $\text{NICS}_{zz}(0)$ and $\text{NICS}_{zz}(1)$ values calculated for each B_3 triangle in D_{3h} $\text{B}_{18}\text{H}_3^-$ (**6**), C_s $\text{B}_{18}\text{H}_3^-$ (**15**), D_{2h} B_{18}H_4 (**8**), C_{2v} $\text{B}_{18}\text{H}_5^+$ (**10**), and D_{6h} $\text{B}_{18}\text{H}_6^{2+}$ (**12**) at B3LYP level

	AMS	$\text{NICS}_{zz}(0)$	$\text{NICS}_{zz}(1)$
 B_{18}H_2 $C_{2v} ({}^1A_1)$	-378.7	a	-55.4
		b	-52.0
		c	-71.0
		d	-55.0
		e	-51.8
		f	-100.5
 $\text{B}_{18}\text{H}_3^-$ $D_{3h} ({}^1A_1)$	-518.0	a	-30.5
		b	-47.7
		c	-77.2
		d	-60.3
 $\text{B}_{18}\text{H}_3^-$ $C_s ({}^1A)$	-505.9	a	-29.3
		b	-47.7
		c	-76.0
		d	-59.9
		e	-60.4
		f	-77.0
		g	-48.4
		h	-48.8
		i	-76.3
		j	-59.9
 B_{18}H_4 $D_{2h} ({}^1A_g)$	-450.5	a	-6.6
		b	-57.4
		c	-74.8
		d	-55.7
		e	-51.9
		f	-80.2

	AMS	NICS _{zz} (0)	NICS _{zz} (1)	
 $B_{18}H_5^+$ $C_{2v} (^1A_1)$		-14.1	-30.9	
	a		-14.1	-30.9
	b		-55.6	-31.9
	c		-79.0	-45.4
	d		-53.6	-31.2
	e	-433.0	-56.7	-33.2
	f		-79.7	-47.8
	g		-49.1	-33.0
	h		-58.5	-33.6
	i		-72.9	-50.2
j		-55.0	-33.0	
 $B_{18}H_6^{2+}$ $D_{6h} (^1A_{1g})$		-20.2	-32.5	
	a		-20.2	-32.5
	b	-403.3	-55.9	-30.9
c		-77.6	-45.0	