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Electronic Supplementary Information:

Photoelectron spectroscopy of aromatic compound clusters of the B_{12} all-boron benzene: $B_{12}Au^-$ and $B_{12}(BO)^-$†

Hui Bai,[a] Hua-Jin Zhai,[ab] Si-Dian Li,[a] and Lai-Sheng Wang[b]

[a] *Institute of Molecular Science, Shanxi University, Taiyuan 030006, China*

[b] *Department of Chemistry, Brown University, Providence, Rhode Island 02912, United States*

Table S1. Analysis of the occupied molecular orbitals (MOs) for the B_{12}^- (C_s, $^2A'$), $B_{12}H^-$ (**31**, C_1, ^1A), $B_{12}Au^-$ (**1**, C_1, ^1A), and $B_{13}O^-$ (**16**, C_1, ^1A) clusters. The MOs are depicted in Figures S6–S8.

Table S2. Vibrational frequencies of the (C_1, ^2A) ground-state structures of $B_{12}Au$ (**13**), $B_{12}(BO)$ (**28**), and $B_{12}H$ (**43**) calculated at the B3LYP/6-311G(d,p) level.

Table S3. Cartesian coordinates and the total energies (in a.u.) at the B3LYP/6-311G(d,p) level for anion global minima (**1** for $B_{12}Au^-$ and **16** for $B_{13}O^-$) and low-lying structures (**2** and **3** for $B_{12}Au^-$; **17** and **18** for $B_{13}O^-$) and their corresponding neutral structures (**13**–**15** for $B_{12}Au$ and **28**–**30** for $B_{13}O$).

Figures S1–S3. Optimized anion cluster structures for $B_{12}Au^-$ (**1**–**12**), $B_{13}O^-$ (**16**–**27**), and $B_{12}H^-$ (**31**–**42**), and their selected neutral structures (**13**–**15**, **28**–**30**, and **43**–**46**) at the B3LYP level. The lowest vibrational frequency (ν_{min}) and relative energy (ΔE) are labeled under each structure. Relative energies of the four lowest energy anion isomers at single-point CCSD(T) level are shown in square brackets.

Figure S4. Comparison of the potential energy surfaces of $B_{12}H^-$, $B_{12}Au^-$, and $B_{13}O^-$ clusters.

Figure S5. Simulated photoelectron spectra based on the C_1 global minimum structures of $B_{12}H^-$ (**31**), $B_{12}Au^-$ (**1**), and $B_{13}O^-$ (**16**) clusters. The simulations were done by fitting the distribution of the calculated vertical detachment energies with unit-area Gaussian functions of 0.05 eV halfwidth.

Figures S6–S8. Occupied molecular orbitals for B_{12}^- (C_s, $^2A'$), $B_{12}H^-$ (**31**), $B_{12}Au^-$ (**1**), and $B_{13}O^-$ (**16**) clusters.

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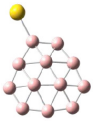
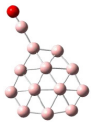
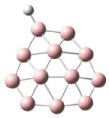
Table S1. Analysis of the occupied molecular orbitals (MOs) for the B_{12}^- (C_s, $^2A'$), $B_{12}H^-$ (**31**, C_1, ^1A), $B_{12}Au^-$ (**1**, C_1, ^1A), and $B_{13}O^-$ (**16**, C_1, ^1A) clusters. The MOs are depicted in Figures S6–S8.

$B_{12}X^-$	B_{12}^-	$B_{12}H^-$	$B_{12}Au^-$	$B_{12}(BO)^-$
Bonds or lone-pairs in X			***Au d^{10} lone-pairs***:	***B≡O triple bond***:
			HOMO-5 (a)	HOMO-9 (a)
			HOMO-7 (a)	HOMO-10 (a)
			HOMO-8 (a)	HOMO-14 (a)
			HOMO-9 (a)	
			HOMO-13 (a)	***O 2s lone-pair***:
				HOMO-22 (a)
SOMO or X-B_{12} single bond	SOMO (a′)	HOMO-11 (a)	HOMO (a)	HOMO-15 (a)
Peripheral B-B σ bonds	HOMO-8 (a′)	HOMO-6 (a)	HOMO-12 (a)	HOMO-5 (a)
(***nine 2c-2e σ bonds***)	HOMO-9 (a′)	HOMO-9 (a)	HOMO-15 (a)	HOMO-8 (a)
	HOMO-11 (a″)	HOMO-10 (a)	HOMO-16 (a)	HOMO-12 (a)
	HOMO-12 (a′)	HOMO-13 (a)	HOMO-17 (a)	HOMO-13 (a)
	HOMO-14 (a′)	HOMO-14 (a)	HOMO-19 (a)	HOMO-17 (a)
	HOMO-15 (a′)	HOMO-15 (a)	HOMO-20 (a)	HOMO-18 (a)
	HOMO-16 (a″)	HOMO-16 (a)	HOMO-21 (a)	HOMO-19 (a)
	HOMO-17 (a′)	HOMO-17 (a)	HOMO-22 (a)	HOMO-20 (a)
	HOMO-18 (a′)	HOMO-18 (a)	HOMO-23 (a)	HOMO-21 (a)
Inner triangle B-B σ bonds	HOMO-6 (a′)	HOMO-5 (a)	HOMO-10 (a)	HOMO-6 (a)
(***three σ bonds***)[a]	HOMO-7 (a″)	HOMO-7 (a)	HOMO-11 (a)	HOMO-7 (a)
	HOMO-13 (a″)	HOMO-12 (a)	HOMO-18 (a)	HOMO-16 (a)
Delocalized σ orbitals	HOMO-1 (a″)	HOMO (a)	HOMO-1 (a)	HOMO (a)
(***six σ electrons***; $4n + 2$)	HOMO-2 (a′)	HOMO-1 (a)	HOMO-2 (a)	HOMO-1 (a)
	HOMO-5 (a″)	HOMO-4 (a)	HOMO-6 (a)	HOMO-4 (a)
Delocalized π orbitals	HOMO-3 (a″)	HOMO-2 (a)	HOMO-3 (a)	HOMO-2 (a)
(***six π electrons***; $4n + 2$)	HOMO-4 (a′)	HOMO-3 (a)	HOMO-4 (a)	HOMO-3 (a)
	HOMO-10 (a′)	HOMO-8 (a)	HOMO-14 (a)	HOMO-11 (a)

[a] Tentative and rough assignment. AdNDP analyses reach a slightly different conclusion; see Fig. 5 and the text.

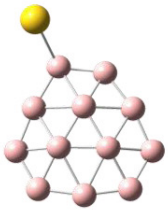
Table S2. Vibrational frequencies of the (C_1, ^{2}A) ground-state structures of $B_{12}Au$ (**13**), $B_{12}(BO)$ (**28**), and $B_{12}H$ (**43**) calculated at the B3LYP/6-311G(d,p) level.

ω_i	$B_{12}Au$ (**13**) 	$B_{12}(BO)$ (**28**) 	$B_{12}H$ (**43**) 
ω_1	1323(a)	1995(a)[a]	2601(a)[a]
ω_2	1263(a)	1331(a)	1328(a)
ω_3	1233(a)	1263(a)	1258(a)
ω_4	1162(a)	1227(a)	1227(a)
ω_5	1147(a)	1177(a)	1165(a)
ω_6	1111(a)	1142(a)	1146(a)
ω_7	1087(a)	1130(a)	1095(a)
ω_8	946(a)	1067(a)	1061(a)
ω_9	932(a)	997(a)	945(a)
ω_{10}	909(a)	927(a)	920(a)
ω_{11}	858(a)	889(a)	895(a)
ω_{12}	814(a)	842(a)	829(a)
ω_{13}	694(a)[b]	816(a)	803(a)
ω_{14}	663(a)	729(a)	743(a)
ω_{15}	623(a)	687(a)[b]	676(a)[b]
ω_{16}	599(a)	635(a)	655(a)
ω_{17}	577(a)	610(a)	642(a)
ω_{18}	554(a)	593(a)	617(a)
ω_{19}	519(a)	564(a)	603(a)
ω_{20}	502(a)	542(a)	582(a)
ω_{21}	498(a)	504(a)	527(a)
ω_{22}	470(a)	496(a)	500(a)
ω_{23}	452(a)	468(a)	476(a)
ω_{24}	441(a)	456(a)	470(a)
ω_{25}	402(a)	445(a)	450(a)
ω_{26}	376(a)	428(a)	426(a)
ω_{27}	363(a)	404(a)	414(a)
ω_{28}	262(a)	389(a)	390(a)
ω_{29}	214(a)	359(a)	362(a)
ω_{30}	193(a)	335(a)	336(a)
ω_{31}	147(a)[a]	321(a)	219(a)
ω_{32}	62(a)	229(a)	191(a)
ω_{33}	40(a)	196(a)	175(a)
ω_{34}		182(a)	
ω_{35}		71(a)	
ω_{36}		69(a)	

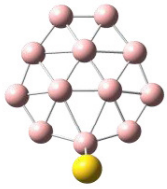
[a] B-Au stretching; B≡O stretching; B-H stretching.

[b] B_{12} breathing.

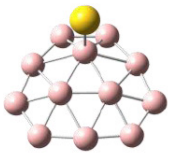
Figure S1. Optimized structures for $B_{12}Au^-$ (**1–12**) and $B_{12}Au$ (**13–15**) at the B3LYP level. The lowest vibrational frequency (ν_{min}) and relative energy (ΔE) are labeled under each structure. Relative energy of the four lowest energy anion isomers at single-point CCSD(T) level is shown in square brackets. Structure **14** is a first order saddle point.



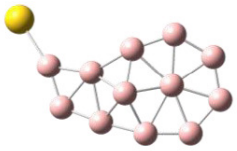
1. C_1 (^1A) $B_{12}Au^-$
ν_{min} = +63 cm^{-1}
ΔE = 0.00 kcal/mol
[0.00 kcal/mol]



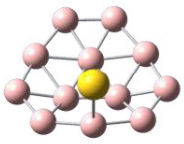
2. C_s ($^1A'$) $B_{12}Au^-$
ν_{min} = +57 cm^{-1}
ΔE = +1.24 kcal/mol
[+0.39 kcal/mol]



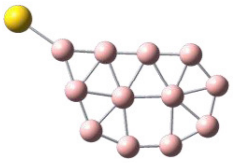
3. C_s ($^1A'$) $B_{12}Au^-$
ν_{min} = +66 cm^{-1}
ΔE = +6.55 kcal/mol
[+0.51 kcal/mol]



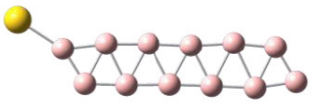
4. C_1 (^1A) $B_{12}Au^-$
ν_{min} = +46 cm^{-1}
ΔE = +9.13 kcal/mol
[+10.13 kcal/mol]



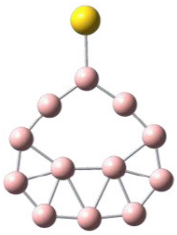
5. C_s ($^1A'$) $B_{12}Au^-$
ν_{min} = +48 cm^{-1}
ΔE = +11.55 kcal/mol



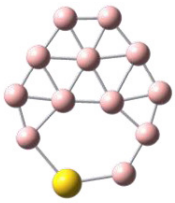
6. C_1 (^1A) $B_{12}Au^-$
ν_{min} = +15 cm^{-1}
ΔE = +12.66 kcal/mol



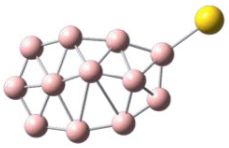
7. C_s ($^1A'$) $B_{12}Au^-$
ν_{min} = +40 cm^{-1}
ΔE = +15.04 kcal/mol



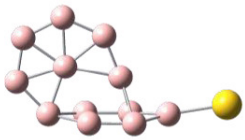
8. C_{2v} ($^1A_1$) $B_{12}Au^-$
ν_{min} = +41 cm^{-1}
ΔE = +15.08 kcal/mol



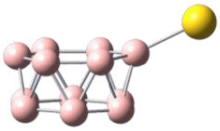
9. C_s ($^1A'$) $B_{12}Au^-$
ν_{min} = +82 cm^{-1}
ΔE = +23.65 kcal/mol



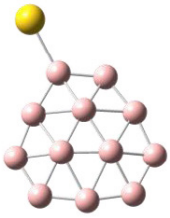
10. C_1 (^1A) $B_{12}Au^-$
ν_{min} = +63 cm^{-1}
ΔE = +27.29 kcal/mol



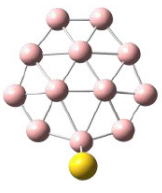
11. C_s ($^1A'$) $B_{12}Au^-$
ν_{min} = +44 cm^{-1}
ΔE = +30.59 kcal/mol



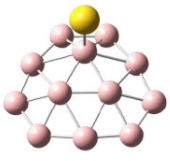
12. C_s ($^1A'$) $B_{12}Au^-$
ν_{min} = +98 cm^{-1}
ΔE = +51.77 kcal/mol



13. C_1 (^2A) $B_{12}Au$
ν_{min} = +40 cm^{-1}
ΔE = 0.00 kcal/mol

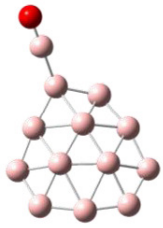


14. C_s ($^2A'$) $B_{12}Au$
ν_{min} = −83 cm^{-1}
ΔE = +10.53 kcal/mol

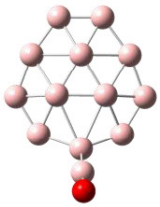


15. C_s ($^2A'$) $B_{12}Au$
ν_{min} = +59 cm^{-1}
ΔE = +13.52 kcal/mol

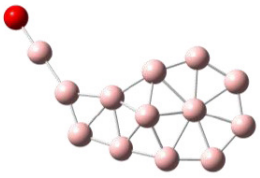
Figure S2. Optimized structures for $B_{13}O^-$ (**16**–**27**) and $B_{13}O$ (**28**–**30**) at the B3LYP level. The lowest vibrational frequency (ν_{min}) and relative energy (ΔE) are labeled under each structure. Relative energy of the four lowest energy anion isomers at single-point CCSD(T) level is shown in square brackets. Number of imaginary frequencies is also shown in parentheses for structure **26**, which is a second order saddle point.



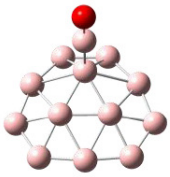
16. C_1 (^{1}A) $B_{12}(BO)^-$
ν_{min} = +76 cm^{-1}
ΔE = 0.00 kcal/mol
[0.00 kcal/mol]



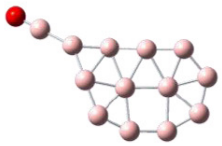
17. C_s (^{1}A′) $B_{12}(BO)^-$
ν_{min} = +77 cm^{-1}
ΔE = +2.96 kcal/mol
[+2.81 kcal/mol]



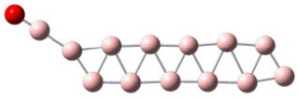
18. C_1 (^{1}A) $B_{12}(BO)^-$
ν_{min} = +54 cm^{-1}
ΔE = –0.27 kcal/mol
[+3.38 kal/mol]



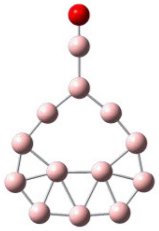
19. C_s (^{1}A′) $B_{12}(BO)^-$
ν_{min} = +86 cm^{-1}
ΔE = +11.16 kcal/mol
[+8.47 kcal/mol]



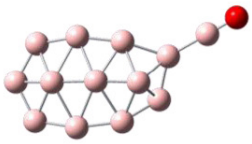
20. C_1 (^{1}A) $B_{12}(BO)^-$
ν_{min} = +38 cm^{-1}
ΔE = +6.88 kcal/mol



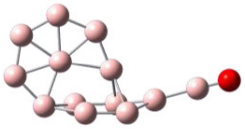
21. C_1 (^{1}A) $B_{12}(BO)^-$
ν_{min} = +41 cm^{-1}
ΔE = +10.42 kcal/mol



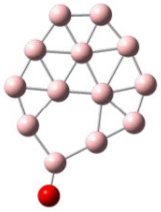
22. C_{2v} (^{1}A$_1$) $B_{12}(BO)^-$
ν_{min} = +48 cm^{-1}
ΔE = +10.47 kcal/mol



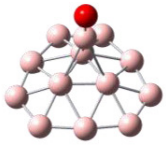
23. C_1 (^{1}A) $B_{12}(BO)^-$
ν_{min} = +76 cm^{-1}
ΔE = +20.63 kcal/mol



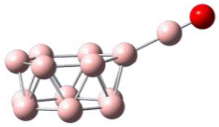
24. C_s (^{1}A′) $B_{12}(BO)^-$
ν_{min} = +76 cm^{-1}
ΔE = +20.63 kcal/mol



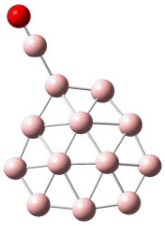
25. C_s (^{1}A′) $B_{12}(BO)^-$
ν_{min} = +46 cm^{-1}
ΔE = +40.11 kcal/mol



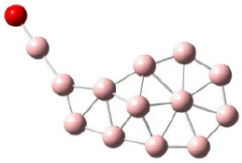
26. C_{3v} (^{1}A$_1$) $B_{12}(BO)^-$
ν_{min} = –428(2) cm^{-1}
ΔE = +46.00 kcal/mol



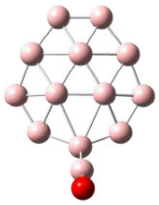
27. C_s (^{1}A′) $B_{12}(BO)^-$
ν_{min} = +95 cm^{-1}
ΔE = +48.24 kcal/mol



28. C_1 (^{2}A) $B_{12}(BO)$
ν_{min} = +69 cm^{-1}
ΔE = 0.00 kcal/mol

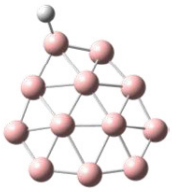


29. C_1 (^{2}A) $B_{12}(BO)$
ν_{min} = +53 cm^{-1}
ΔE = +3.59 kcal/mol

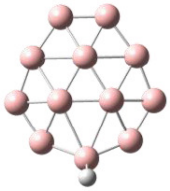


30. C_s (^{2}A′) $B_{12}(BO)$
ν_{min} = +68 cm^{-1}
ΔE = +17.80 kcal/mol

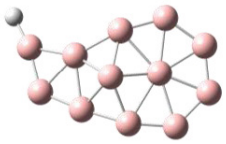
Figure S3. Optimized structures for $B_{12}H^-$ (**31**–**42**) and $B_{12}H$ (**43**–**46**) at the B3LYP level. The lowest vibrational frequency (ν_{min}) and relative energy (ΔE) are labeled under each structure. Relative energy of the four lowest energy anion isomers at single-point CCSD(T) level is shown in square brackets. Number of imaginary frequencies is also shown in parentheses for structure **40**, which is a second order saddle point.



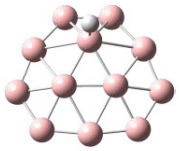
31. C_1 (^{1}A) $B_{12}H^-$
ν_{min} = +185 cm^{-1}
ΔE = 0.00 kcal/mol
[0.00 kcal/mol]



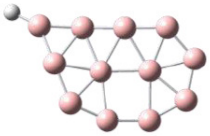
32. C_s (^{1}A′) $B_{12}H^-$
ν_{min} = +183 cm^{-1}
ΔE = +0.24 kcal/mol
[+0.71 kcal/mol]



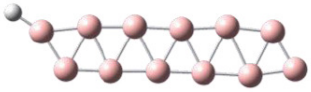
33. C_1 (^{1}A) $B_{12}H^-$
ν_{min} = +104 cm^{-1}
ΔE = +1.26 kcal/mol
[+3.46 kcal/mol]



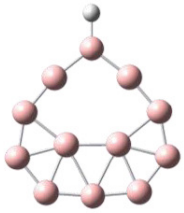
34. C_s (^{1}A′) $B_{12}H^-$
ν_{min} = +187 cm^{-1}
ΔE = +7.01 kcal/mol
[+5.54 kcal/mol]



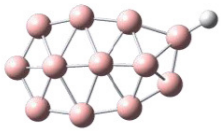
35. C_1 (^{1}A) $B_{12}H^-$
ν_{min} = +56 cm^{-1}
ΔE = +7.74 kcal/mol



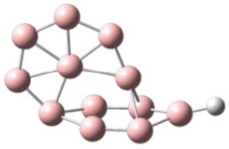
36. C_1 (^{1}A) $B_{12}H^-$
ν_{min} = +66 cm^{-1}
ΔE = +9.04 kcal/mol



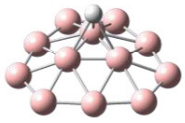
37. C_{2v} (^{1}A$_1$) $B_{12}H^-$
ν_{min} = +71 cm^{-1}
ΔE = +11.13 kcal/mol



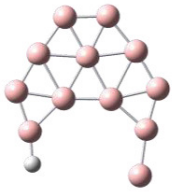
38. C_1 (^{1}A) $B_{12}H^-$
ν_{min} = +154 cm^{-1}
ΔE = +22.00 kcal/mol



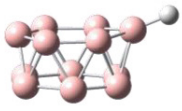
39. C_s (^{1}A′) $B_{12}H^-$
ν_{min} = +65 cm^{-1}
ΔE = +23.85 kcal/mol



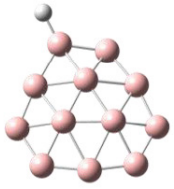
40. C_{3v} (^{1}A$_1$) $B_{12}H^-$
ν_{min} = –802(2) cm^{-1}
ΔE = +42.40 kcal/mol



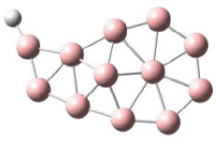
41. C_s (^{1}A′) $B_{12}H^-$
ν_{min} = +70 cm^{-1}
ΔE = +48.02 kcal/mol



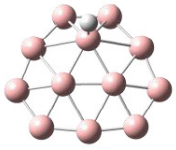
42. C_s (^{1}A′) $B_{12}H^-$
ν_{min} = +192 cm^{-1}
ΔE = +50.00 kcal/mol



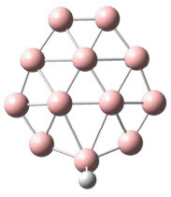
43. C_1 (^{2}A) $B_{12}H$
ν_{min} = +175 cm^{-1}
ΔE = 0.00 kcal/mol



44. C_1 (^{2}A) $B_{12}H$
ν_{min} = +103 cm^{-1}
ΔE = +4.11 kcal/mol



45. C_s (^{2}A′) $B_{12}H$
ν_{min} = +109 cm^{-1}
ΔE = +11.64 kcal/mol



46. C_s (^{2}A′) $B_{12}H$
ν_{min} = +158 cm^{-1}
ΔE = +16.80 kcal/mol

Figure S4. Comparison of the potential energy surfaces of $B_{12}H^-$, $B_{12}Au^-$, and $B_{13}O^-$ clusters. The relative energies are at the single-point CCSD(T) level and the isomers are numbered the same as in Fig. 3 and Figs. S1–S3.

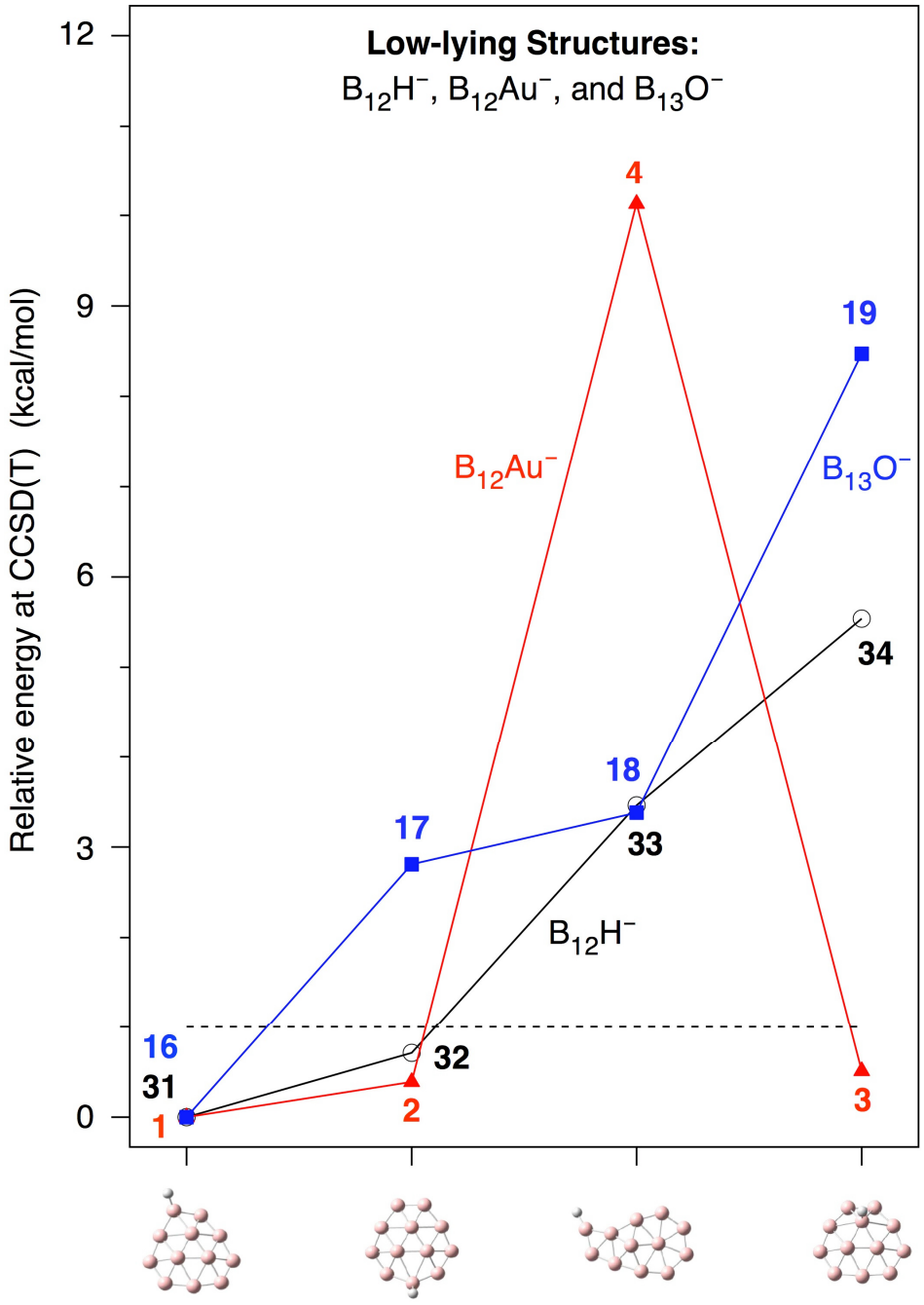


Figure S5. Simulated photoelectron spectra based on the C_1 global minimum structures of $B_{12}H^-$ (**31**), $B_{12}Au^-$ (**1**), and $B_{13}O^-$ (**16**) clusters. The simulations were done by fitting the distribution of the calculated vertical detachment energies with unit-area Gaussian functions of 0.05 eV halfwidth.

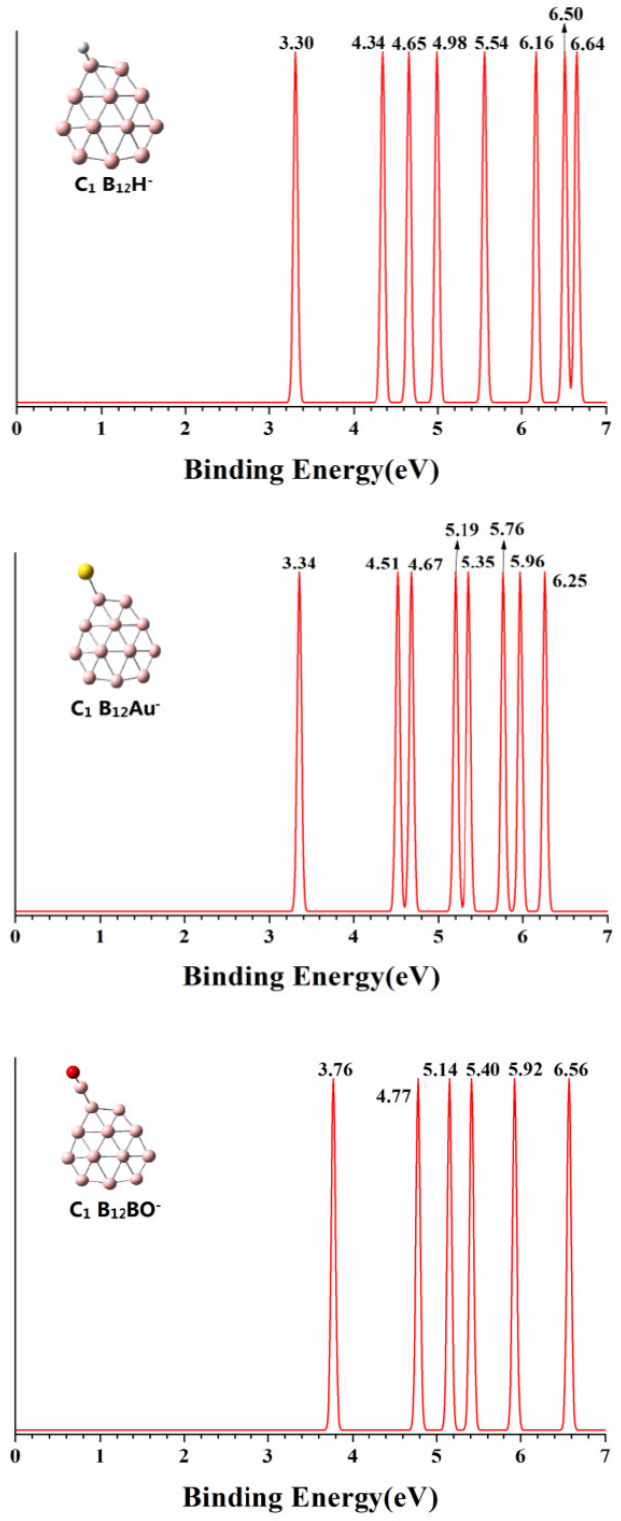


Figure S6. Occupied molecular orbitals for B_{12}^- (C_s, $^2A'$).

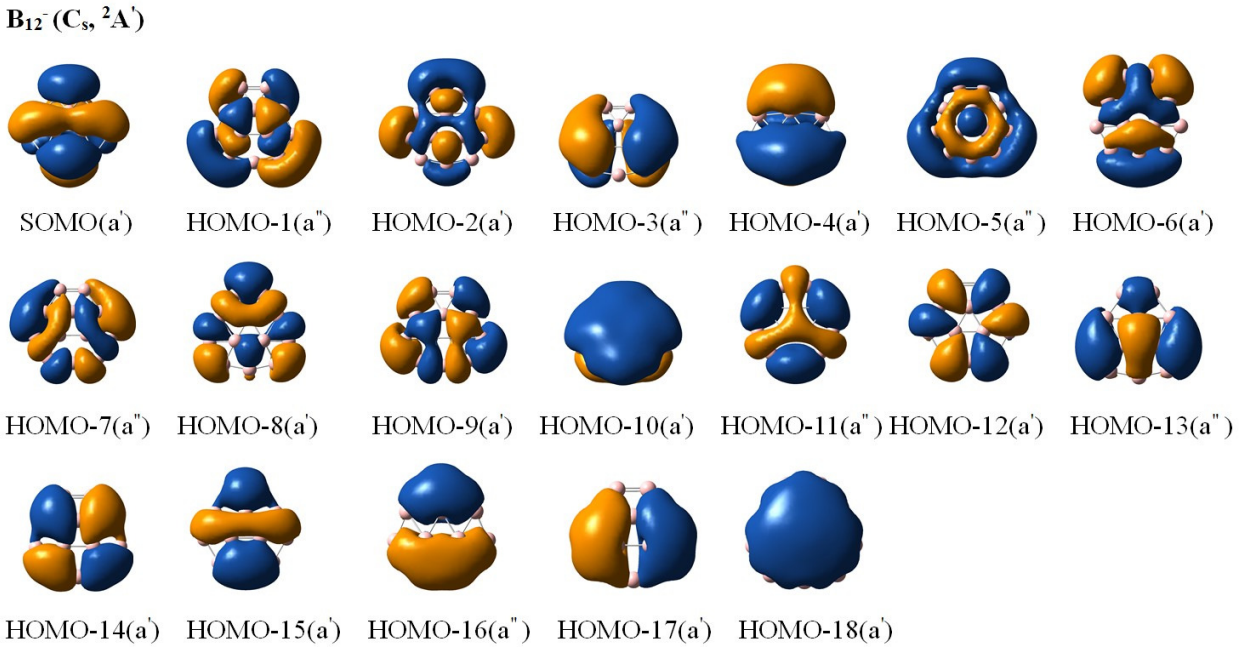


Figure S7. Occupied molecular orbitals for $B_{12}H^-$ (C_1, ^1A).

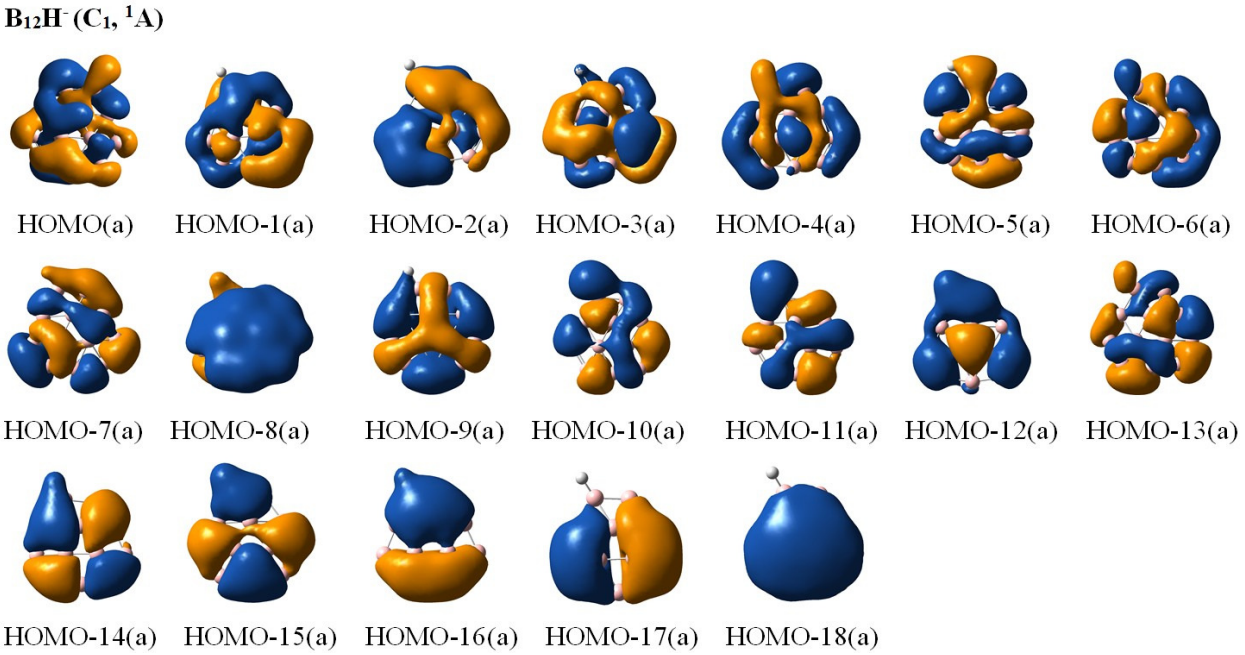


Figure S8. Occupied molecular orbitals for (a) $B_{12}Au^-$ (C_1, ^1A) and (b) $B_{12}(BO)^-$ (C_1, ^1A).

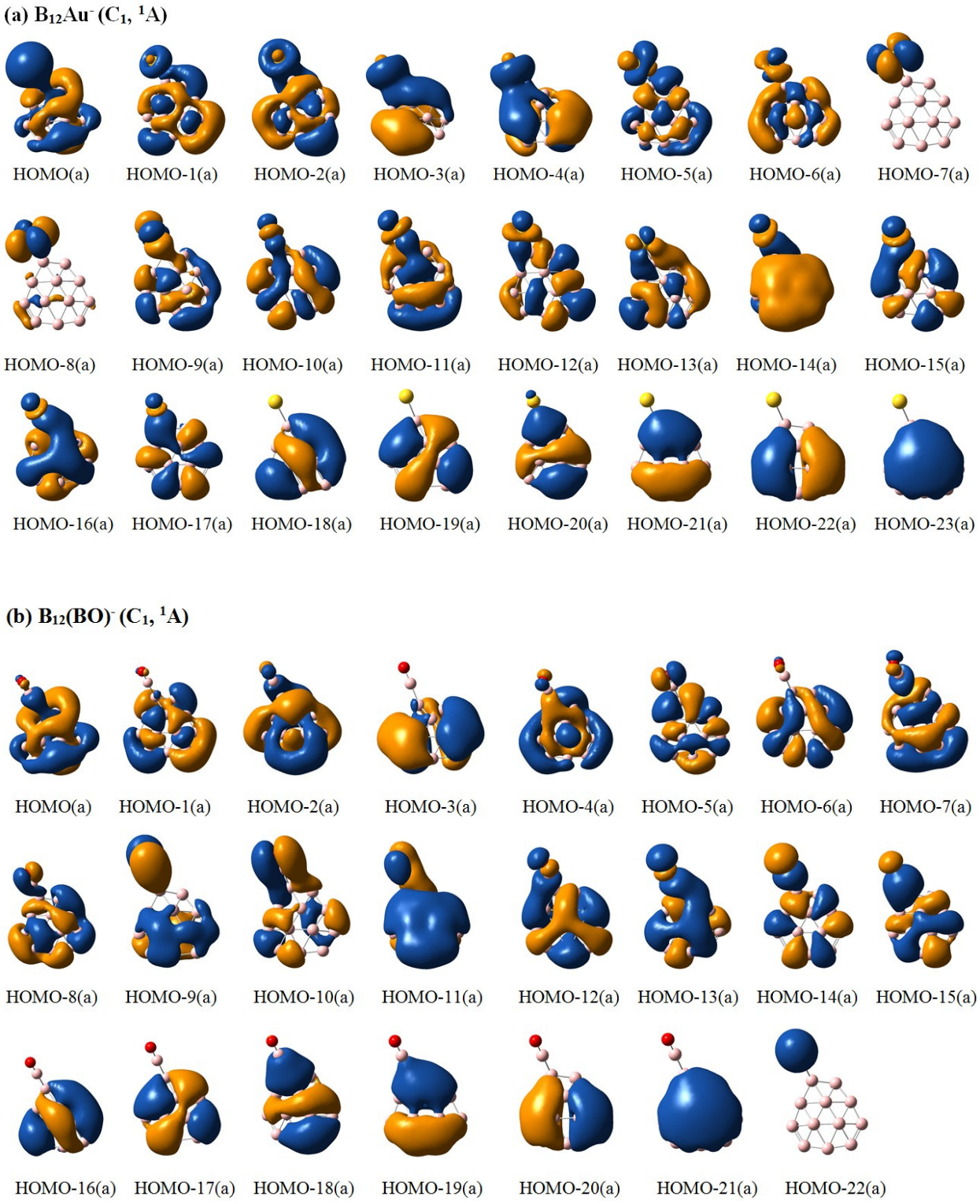


Table S3. Cartesian coordinates and the total energies (in a.u.) at the B3LYP/6-311G(d,p) level for anion global minima (**1** for $B_{12}Au^-$ and **16** for $B_{13}O^-$) and low-lying structures (**2** and **3** for $B_{12}Au^-$; **17** and **18** for $B_{13}O^-$) and their corresponding neutral structures (**13**–**15** for $B_{12}Au$ and **28**–**30** for $B_{13}O$).

1. C_1 $B_{12}Au^-$

Total energy=-434.0880699a.u.

Atomic Number	X	Y	Z
5	4.373936	0.761290	-0.404336
5	2.281914	-1.932103	0.311190
5	1.014743	1.179813	0.650628
5	1.540109	-0.393081	-0.060916
5	3.150060	-0.609531	-0.531864
5	2.518369	0.938021	-0.263204
5	3.619374	2.128007	-0.003891
5	2.168974	2.313690	0.520263
5	0.010267	-0.141393	0.743891
5	0.815414	-1.532762	0.866794
5	3.880232	-1.977687	0.003493
5	4.781624	-0.770022	-0.374971
79	-1.908545	0.002263	-0.092220

2. C_s $B_{12}Au^-$

Total energy=-434.0860913a.u.

Atomic Number	X	Y	Z
5	0.930966	0.080419	0.000000
5	-0.136021	3.255803	1.727524
5	-0.136021	3.255803	-1.727524
5	-0.568033	3.061591	0.000000
5	-0.038458	1.709956	0.850679
5	-0.038458	1.709956	-0.850679
5	1.122981	0.729538	-1.503235
5	0.641675	1.975254	-2.297129
5	-0.613994	4.492917	-0.770063
5	-0.613994	4.492917	0.770063
5	0.641675	1.975254	2.297129
5	1.122981	0.729538	1.503235
79	-0.146538	-1.738541	0.000000

3. C_s $B_{12}Au^-$

Total energy=-434.0776283a.u.

Atomic Number	X	Y	Z
5	0.804997	0.602209	0.000000
5	-0.056795	2.152052	2.353338
5	-0.056795	2.152052	-2.353338
5	-1.275474	2.701357	1.580511
5	-1.275474	2.701357	-1.580511
5	2.354759	0.962302	0.763011
5	-0.367829	1.537691	-0.847112

5	-1.523892	2.657981	0.000000
5	-0.367829	1.537691	0.847112
5	1.210959	1.382302	1.773009
5	1.210959	1.382302	-1.773009
5	2.354759	0.962302	-0.763011
79	-0.190655	-1.312127	0.000000

13. $C_1 B_{12}Au$

Total energy=-433.9718797a.u.

Atomic Number	X	Y	Z
5	4.469491	0.786876	-0.103560
5	2.344227	-1.981999	0.137624
5	1.017295	1.196873	0.242466
5	1.620251	-0.369922	-0.257730
5	3.307289	-0.593284	-0.433040
5	2.647846	0.948672	-0.339356
5	3.660350	2.166337	0.115533
5	2.128782	2.358207	0.297350
5	0.056916	-0.182812	0.329053
5	0.806970	-1.614299	0.421602
5	3.959873	-1.992174	0.096355
5	4.892163	-0.759271	-0.021173
79	-1.956421	0.002329	-0.030704

14. $C_s B_{12}Au$

Total energy=-433.9550973a.u.

Atomic Number	X	Y	Z
5	0.804631	0.210361	0.000000
5	-0.117032	3.220596	1.754928
5	-0.117032	3.220596	-1.754928
5	-0.486225	3.035774	0.000000
5	-0.092420	1.655819	0.852132
5	-0.092420	1.655819	-0.852132
5	0.949048	0.609760	-1.583039
5	0.491553	1.868450	-2.369918
5	-0.433738	4.480747	-0.775722
5	-0.433738	4.480747	0.775722
5	0.491553	1.868450	2.369918
5	0.949048	0.609760	1.583039
79	-0.121090	-1.703600	0.000000

15. $C_s B_{12}Au$

Total energy=-433.9503413a.u.

Atomic Number	X	Y	Z
5	0.666739	0.567050	0.000000
5	-0.010658	2.177109	2.401652
5	-0.010658	2.177109	-2.401652
5	-1.034400	2.997822	1.591505
5	-1.034400	2.997822	-1.591505
5	2.234892	0.735074	0.771760
5	-0.323785	1.704005	-0.845849
5	-1.238692	3.037460	0.000000

5	-0.323785	1.704005	0.845849
5	1.135999	1.241358	1.815339
5	1.135999	1.241358	-1.815339
5	2.234892	0.735074	-0.771760
79	-0.217224	-1.349066	0.000000

16. C_1 $B_{12}(BO)^-$

Total energy=-398.3161629a.u.

Atomic Number	X	Y	Z
5	2.730575	0.731993	-0.405973
5	0.585022	-1.894994	0.326350
5	-0.630969	1.177219	0.594555
5	-0.139209	-0.380216	-0.142490
5	1.479771	-0.635003	-0.578525
5	0.875835	0.927681	-0.288099
5	1.993743	2.099212	0.001080
5	0.544503	2.289717	0.526284
5	-1.724665	-0.098387	0.571508
5	-0.885940	-1.466294	0.844480
5	2.185227	-1.979213	0.051823
5	3.107683	-0.801709	-0.352488
5	-3.211603	-0.025191	-0.136811
8	-4.318734	0.034490	-0.632308

17. C_s $B_{12}(BO)^-$

Total energy=-398.3114384a.u.

Atomic Number	X	Y	Z
5	-0.683390	1.538125	0.000000
5	0.113325	-1.748830	1.718773
5	0.113325	-1.748830	-1.718773
5	0.582920	-1.558235	0.000000
5	0.125368	-0.180738	0.857461
5	0.125368	-0.180738	-0.857461
5	-1.037647	0.826313	-1.465150
5	-0.646522	-0.447029	-2.257062
5	0.566708	-2.993309	-0.768824
5	0.566708	-2.993309	0.768824
5	-0.646522	-0.447029	2.257062
5	-1.037647	0.826313	1.465150
5	0.292666	2.886771	0.000000
8	0.978337	3.887827	0.000000

18. C_1 $B_{12}(BO)^-$

Total energy=-398.3166008a.u.

Atomic Number	X	Y	Z
5	3.592173	0.488172	-0.590481
5	1.964152	0.331197	0.018923
5	2.851078	1.795350	-0.310801
5	-1.451414	-1.777421	-0.169597
5	-2.394371	-0.601530	-0.035541
5	0.115700	-1.777665	-0.020564
5	3.118005	-0.972804	-0.412379

5	-0.790596	-0.271425	0.319745
5	0.334067	1.001024	0.656687
5	0.778373	-0.540785	0.903484
5	1.752653	-1.567893	0.018617
5	1.424438	2.018907	0.263236
5	-3.723823	0.308750	-0.183483
8	-4.731522	0.978827	-0.286153

28. C_1 B_{12}(BO)

Total energy=-398.1854876a.u.

Atomic Number	X	Y	Z
5	2.762299	0.801823	-0.140455
5	0.655377	-1.968072	0.164184
5	-0.668937	1.172627	0.286542
5	-0.107241	-0.369066	-0.262689
5	1.587566	-0.596519	-0.472265
5	0.925354	0.943622	-0.332799
5	1.947700	2.168653	0.106426
5	0.420783	2.345891	0.335555
5	-1.684623	-0.204303	0.310447
5	-0.872661	-1.615538	0.491171
5	2.264672	-1.975591	0.077667
5	3.184816	-0.741436	-0.070090
5	-3.282711	-0.057003	-0.041447
8	-4.457746	0.059320	-0.282654

29. C_1 B_{12}(BO)

Total energy=-398.1797704a.u.

Atomic Number	X	Y	Z
5	3.672872	0.426370	-0.425723
5	2.001461	0.333904	0.057142
5	2.934678	1.769709	-0.257902
5	-1.458060	-1.788898	-0.164812
5	-2.424485	-0.600178	-0.052205
5	0.117377	-1.780652	-0.027294
5	3.157227	-1.028949	-0.267582
5	-0.791488	-0.197098	0.233728
5	0.291082	1.083935	0.407002
5	0.733404	-0.481619	0.778368
5	1.746648	-1.599247	0.012382
5	1.462817	2.055378	0.142835
5	-3.782897	0.286701	-0.134206
8	-4.787897	0.950403	-0.188584

30. C_s B_{12}(BO)

Total energy=-398.1571161a.u.

Atomic Number	X	Y	Z
5	-0.626932	1.434836	0.000000
5	0.109532	-1.755207	1.753123
5	0.109532	-1.755207	-1.753123
5	0.463140	-1.558739	0.000000
5	0.210027	-0.174477	0.866386

5	0.210027	-0.174477	-0.866386
5	-0.919156	0.854182	-1.520966
5	-0.519851	-0.409060	-2.329659
5	0.428859	-3.018939	-0.779432
5	0.428859	-3.018939	0.779432
5	-0.519851	-0.409060	2.329659
5	-0.919156	0.854182	1.520966
5	0.222244	2.870267	0.000000
8	0.826705	3.912898	0.000000