Structures and bonding of auropolyboroenes $[Au_2(B_4)_xB_3]^-$, $[Au_2(B_4)_xB_2]^{2-}$ and $[Au_2(B_4)_xB]^+$ (x = 2, 3): Comparison with dihydride polyboroenes

Supplementary Information

Peng Shao[a,*], Li-Ping Ding[a], Cheng Lu[b], Jiang-Tao Cai[a], Bo Liu[a] and Chang-Bo Sun[a]

Table S1. Fragmentation channels and dissociation energies (ΔE) for auropolyboroenes $Au_2B_9^+$, $Au_2B_{10}^{2-}$, $Au_2B_{11}^-$, $Au_2B_{13}^+$, $Au_2B_{14}^{2-}$ and $Au_2B_{15}^-$ compared with the corresponding dihydride boron $H_2B_9^+$, $H_2B_{10}^{2-}$, $H_2B_{11}^-$, $H_2B_{13}^+$, $H_2B_{14}^{2-}$ and $H_2B_{15}^-$.

channels	ΔE (eV)
$Au_2B_9^+\left(C_s,{}^1A\right)=AuB_9^+\left(C_s,{}^2A\right)+Au\left(OH,{}^2A_{2g}\right)$	3.53
$H_2B_9^+\left(C_s,{}^1A_1\right)=HB_9^+\left(C_s,{}^2A'\right)+H\left(OH,{}^2A_{2g}\right)$	4.60
$Au_2B_9^+\left(C_s,{}^1A\right)=B_9^+\left(C_2,{}^1A\right)+Au_2\left(D_{\infty h},{}^1\Sigma_g\right)$	4.39
$H_2B_9^+\left(C_s,{}^1A_1\right)=B_9^+\left(C_2,{}^1A\right)+H_2\left(D_{\infty h},{}^1\Sigma_g\right)$	3.18
$Au_2B_{10}^{2-}\left(C_{2h},{}^1A\right)=AuB_{10}^{2-}\left(C_s,{}^2A\right)+Au\left(OH,{}^2A_{2g}\right)$	3.74
$H_2B_{10}^{2-}\left(C_{2h},{}^1A\right)=HB_{10}^{2-}\left(C_s,{}^2A'\right)+H\left(OH,{}^2A_{2g}\right)$	4.56
$Au_2B_{10}^{2-}\left(C_{2h},{}^1A\right)=B_{10}^{2-}\left(D_{2h},{}^1A_g\right)+Au_2\left(D_{\infty h},{}^1\Sigma_g\right)$	4.31
$H_2B_{10}^{2-}\left(C_{2h},{}^1A\right)=B_{10}^{2-}\left(D_{2h},{}^1A_g\right)+H_2\left(D_{\infty h},{}^1\Sigma_g\right)$	3.22

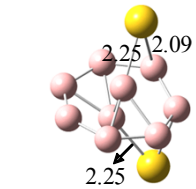
[a] College of Science, Shaanxi University of Science & Technology, Xi'an 710021, China

[b] Department of Physics, Nanyang Normal University, Nanyang 473061, China

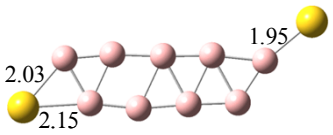
*Correspondence to: Peng Shao, College of Science, Shaanxi University of Science & Technology, Xi'an 710021, China.
E-mail address: scu_sp@163.com (Peng Shao).

$Au_2B_{11}^{-}\left(C_{2v},{}^1A_1\right)=AuB_{11}^{-}\left(C_s,{}^2A'\right)+Au\left(OH,{}^2A_{2g}\right)$	3.50
$H_2B_{11}^{-}\left(C_{2v},{}^1A_1\right)=HB_{11}^{-}\left(C_s,{}^2A'\right)+H\left(OH,{}^2A_{2g}\right)$	4.65
$Au_2B_{11}^{-}\left(C_{2v},{}^1A_1\right)=B_{11}^{-}\left(C_{2v},{}^1A_1\right)+Au_2\left(D_{\infty h},{}^1\Sigma_g\right)$	3.01
$H_2B_{11}^{-}\left(C_{2v},{}^1A_1\right)=B_{11}^{-}\left(C_{2v},{}^1A_1\right)+H_2\left(D_{\infty h},{}^1\Sigma_g\right)$	2.64
$Au_2B_{13}^{+}\left(C_s,{}^1A\right)=AuB_{13}^{+}\left(C_1,{}^2A\right)+Au\left(OH,{}^2A_{2g}\right)$	3.26
$H_2B_{13}^{+}\left(C_{2h},{}^1A\right)=HB_{13}^{+}\left(C_s,{}^2A\right)+H\left(OH,{}^2A_{2g}\right)$	4.64
$Au_2B_{13}^{+}\left(C_s,{}^1A\right)=B_{13}^{+}\left(C_s,{}^1A'\right)+Au_2\left(D_{\infty h},{}^1\Sigma_g\right)$	4.46
$H_2B_{13}^{+}\left(C_{2h},{}^1A\right)=B_{13}^{+}\left(C_s,{}^1A'\right)+H_2\left(D_{\infty h},{}^1\Sigma_g\right)$	2.87
$Au_2B_{14}^{2-}\left(C_{2h},{}^1A\right)=AuB_{14}^{2-}\left(C_s,{}^2A\right)+Au\left(OH,{}^2A_{2g}\right)$	3.65
$H_2B_{14}^{2-}\left(C_{2h},{}^1A_1\right)=HB_{14}^{2-}\left(C_s,{}^2A\right)+H\left(OH,{}^2A_{2g}\right)$	4.58
$Au_2B_{14}^{2-}\left(C_{2h},{}^1A\right)=B_{14}^{2-}\left(C_{2h},{}^1A\right)+Au_2\left(D_{\infty h},{}^1\Sigma_g\right)$	5.40
$H_2B_{14}^{2-}\left(C_{2h},{}^1A_1\right)=B_{14}^{2-}\left(C_{2h},{}^1A\right)+H_2\left(D_{\infty h},{}^1\Sigma_g\right)$	4.54
$Au_2B_{15}^{-}\left(C_{2v},{}^1A\right)=AuB_{15}^{-}\left(C_s,{}^2A\right)+Au\left(OH,{}^2A_{2g}\right)$	3.49
$H_2B_{15}^{-}\left(C_{2h},{}^1A_1\right)=HB_{15}^{-}\left(C_s,{}^1A\right)+H\left(OH,{}^2A_{2g}\right)$	4.65
$Au_2B_{15}^{-}\left(C_{2v},{}^1A\right)=B_{15}^{-}\left(C_1,{}^1A\right)+Au_2\left(D_{\infty h},{}^1\Sigma_g\right)$	3.23
$H_2B_{15}^{-}\left(C_{2h},{}^1A_1\right)=B_{15}^{-}\left(C_1,{}^1A\right)+H_2\left(D_{\infty h},{}^1\Sigma_g\right)$	2.87

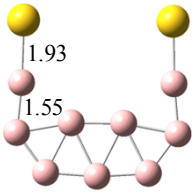
Fig. S1 Optimized structures of the low-lying isomers of $Au_2B_9^+$ and $Au_2B_{10}^{2-}$ auropolyboroenes with their symmetry, electron state and relative energies at B3LYP/Au/SDD/B/6-311+G* method.



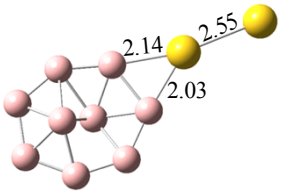
$Au_2B_9^+$–c C_2 ^1A 0.43



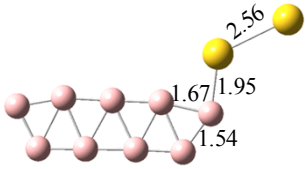
$Au_2B_9^+$–d C_s $^1A'$ 0.45



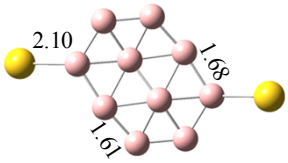
$Au_2B_9^+$–e C_{2v} $^1A_1$ 0.71



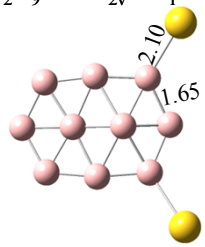
$Au_2B_9^+$–f C_1 ^1A 1.82



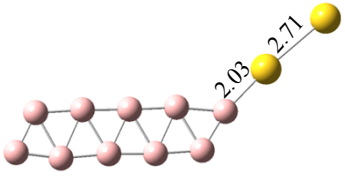
$Au_2B_9^+$–g C_s ^1A 2.27



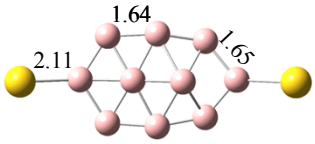
$Au_2B_{10}^{2-}$–c C_i ^1A 0.74



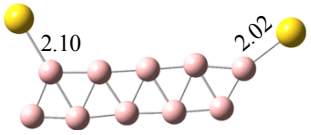
$Au_2B_{10}^{2-}$–d C_s $^1A'$ 0.77



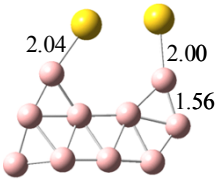
$Au_2B_{10}^{2-}$–e C_s ^1A 1.22



$Au_2B_{10}^{2-}$–f C_1 ^1A 1.54



$Au_2B_{10}^{2-}$–g C_s ^1A 1.78



$Au_2B_{10}^{2-}$–h C_1 ^1A 3.28

Fig. S2 Optimized structures of the low-lying isomers of $Au_2B_{11}^-$ and $Au_2B_{13}^+$ auropolyboroenes with their symmetry, electron state and relative energies at B3LYP/Au/SDD/B/6-311+G* method.

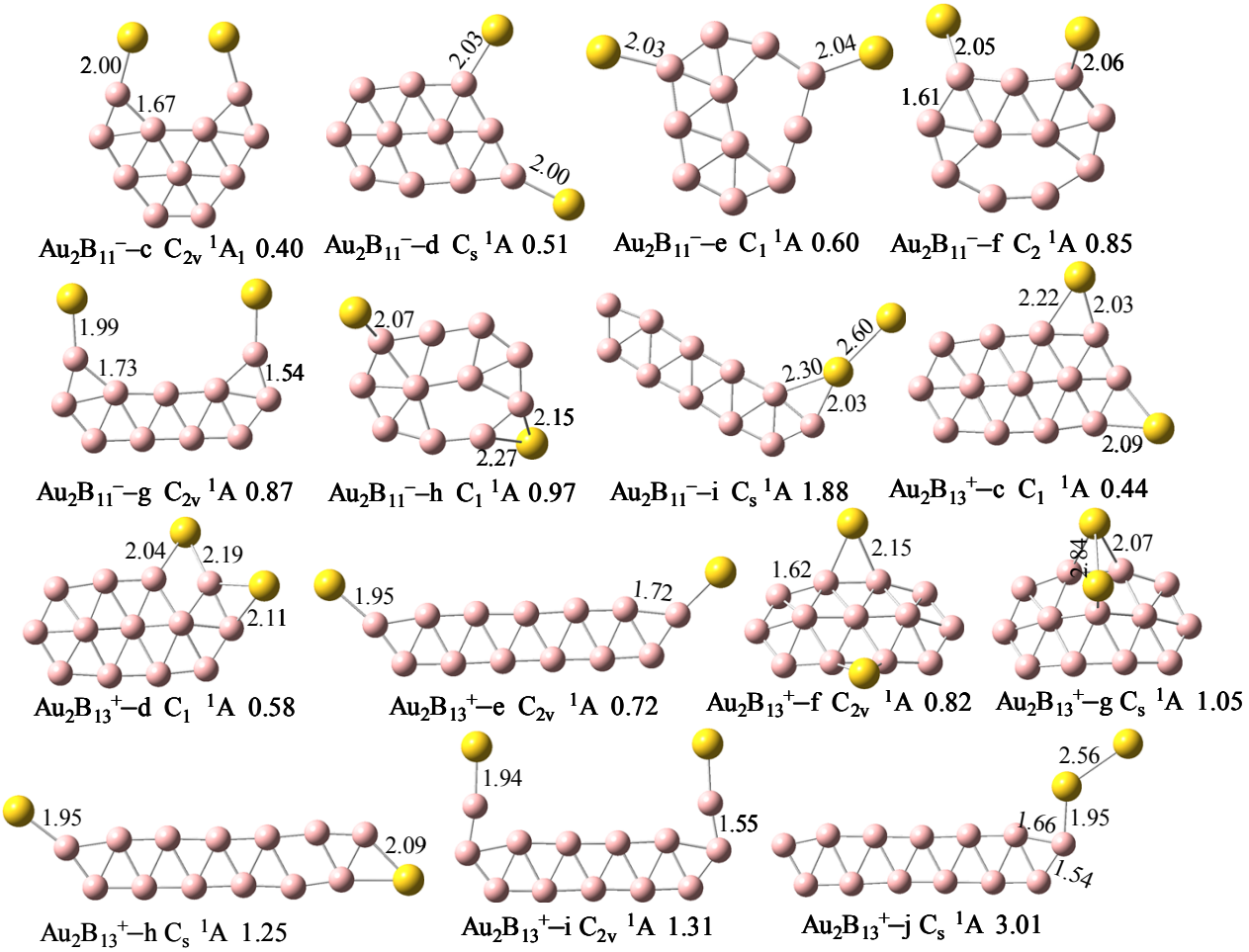


Fig. S3 Optimized structures of the low-lying isomers of $Au_2B_{14}^{2-}$ and $Au_2B_{15}^{-}$ auropolyboroenes with their symmetry, electron state and relative energies at B3LYP/Au/SDD/B/6-311+G* method.

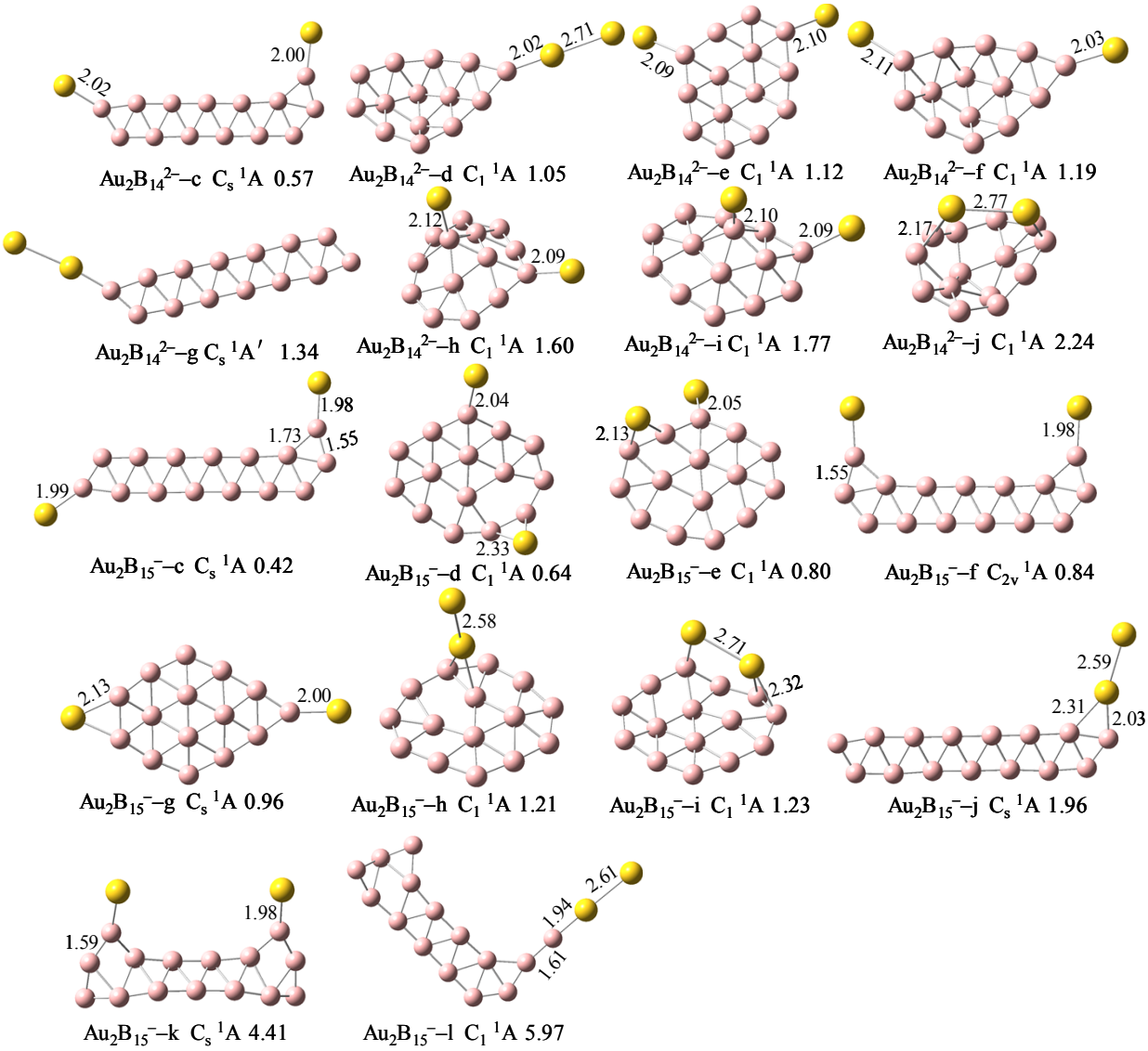


Fig. S4 Optimized lowest-energy structures for dihydride polyboroenes $[H_2(B_4)_xB_3]^-$, $[H_2(B_4)_xB_2]^{2-}$, $[H_2(B_4)_xB]^+$ (x = 2, 3).

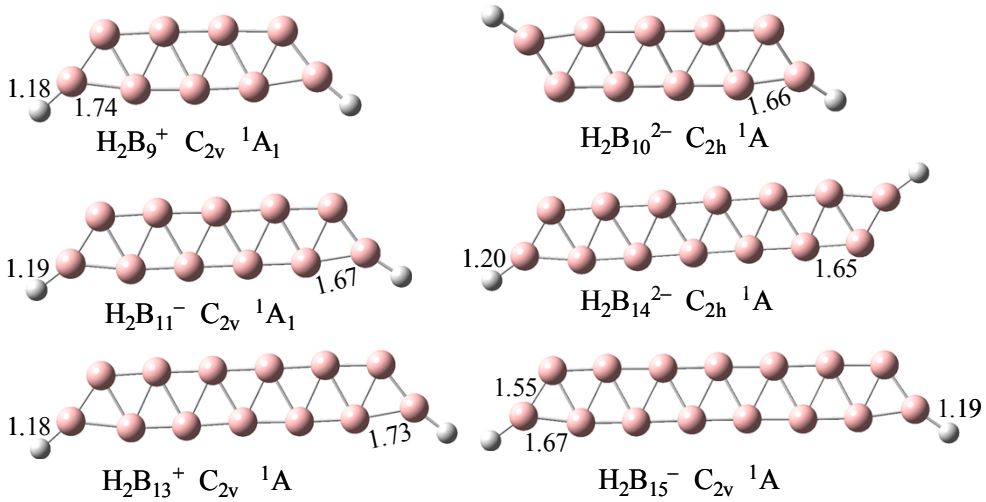


Fig. S5 Optimized the ground state structures of neutral Au_2B_9 and Au_2B_{13} clusters.

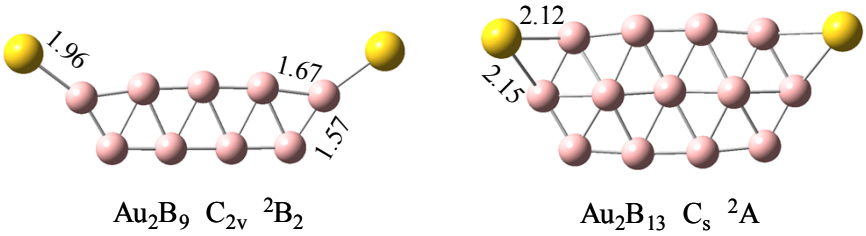


Fig. S6 Chemical bonding analyses for $H_2B_{11}^-$ and $H_2B_{14}^{2-}$ using the AdNDP method.

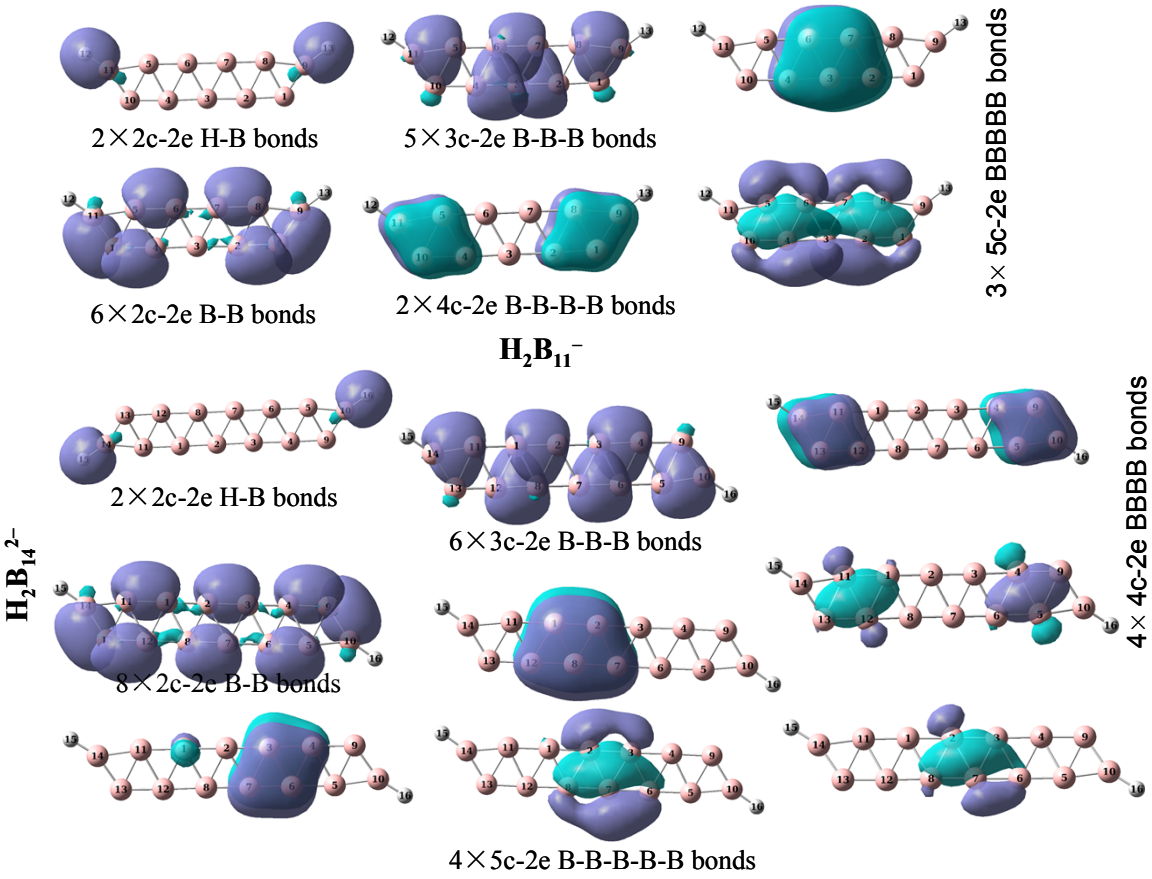


Fig. S7 Simulated photoelectron spectra for the lowest-energy structures of $H_2B_{11}^-$, $Au_2B_{11}^-$ and $Au_2B_{15}^-$ clusters at the TPSS level. Photoelectron spectra of $D_2B_{11}^-$ measured at 266 nm. (The spectra are taken from Ref. 28. Copyright 2012 American Chemical Society).