

## Supporting information

# Lanthanide/actinide boride nanoclusters and nanomaterials based on boron frameworks consisting of conjoined $B_n$ rings ( $n = 7, 8, 9$ )

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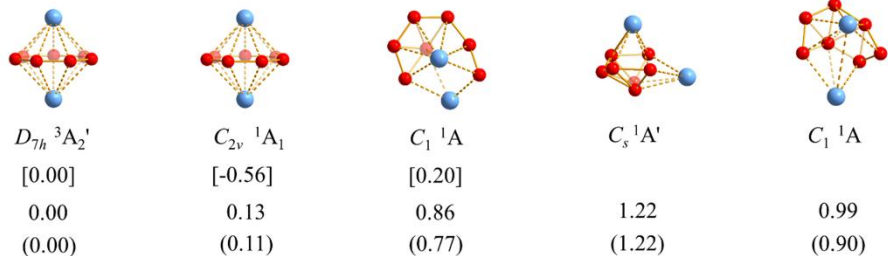
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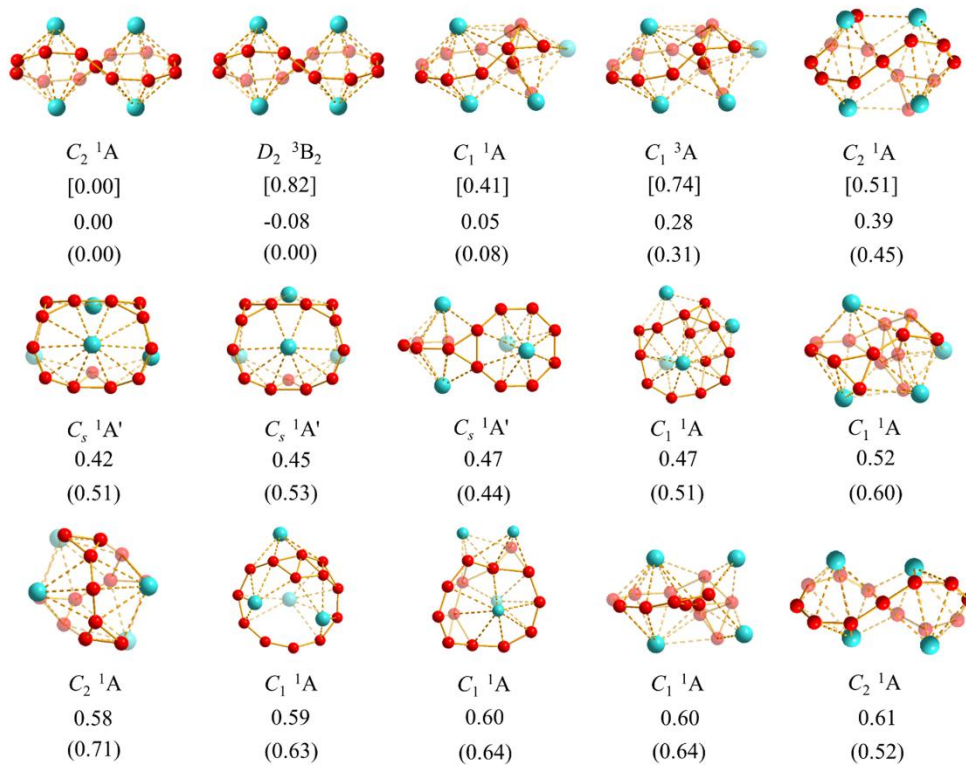
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**Fig. S1** Relative energies of low-lying isomers of  $C_{2v}$   $Ac_2B_7^-$  (**1'**),  $C_2$   $M_4B_{13}^-$  (**2/2'**) (M = La, Ac) at CCSD(T) (square brackets), PBE0, and TPSSh (parentheses) levels in eV.

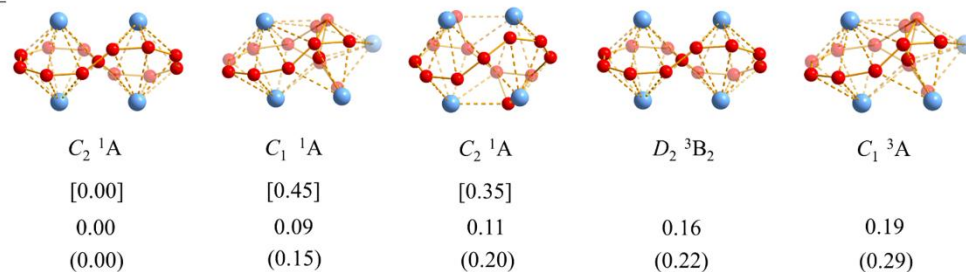
(**1'**)  $Ac_2B_7^-$



(**2**)  $La_4B_{13}^-$

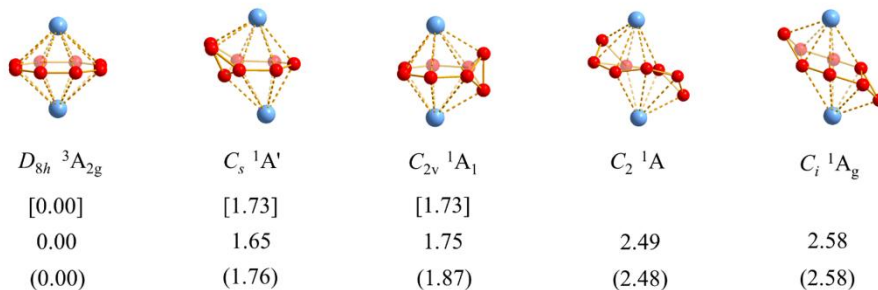


(**2'**)  $Ac_4B_{13}^-$

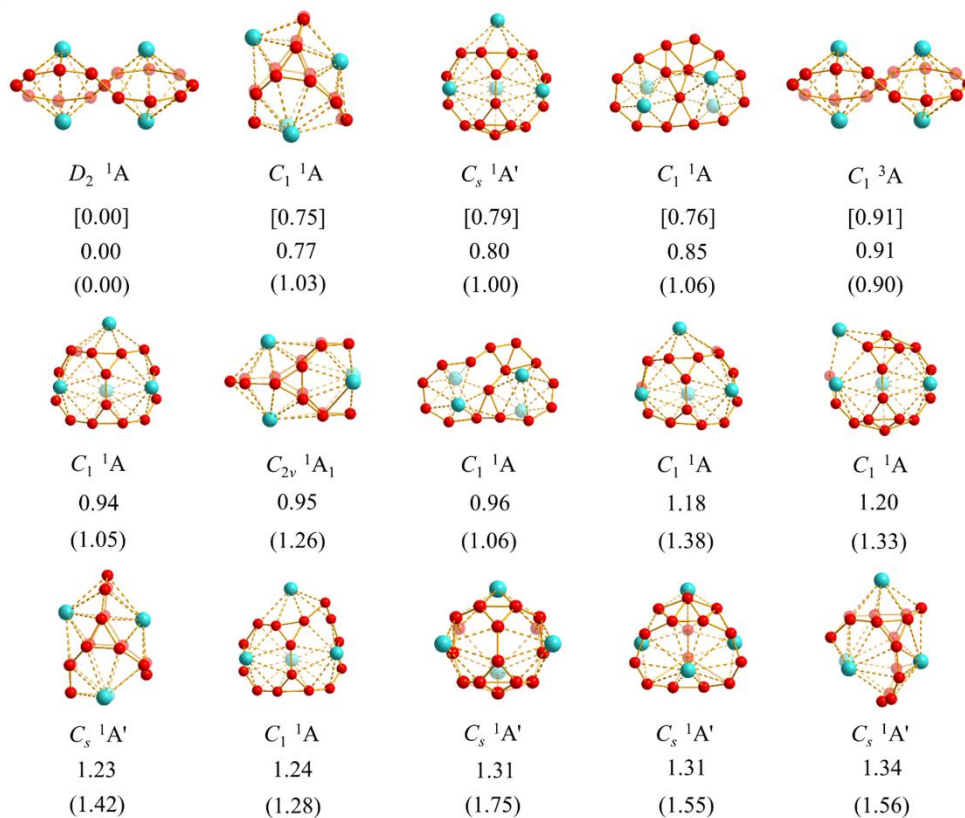


**Fig. S2** Relative energies of low-lying isomers of  $D_{8h}$   $\text{Ac}_2\text{B}_8$  (**3'**),  $D_2$   $\text{M}_4\text{B}_{15}^-$  (**4/4'**),  $C_{3v}/C_3$   $\text{M}_4\text{B}_{18}$  (**5/5'**), and  $O_h$   $\text{Ac}_7\text{B}_{24}^+$  (**6'**) (M = La, Ac) at CCSD(T) (square brackets), PBE0, and TPSSh (parentheses) levels in eV.

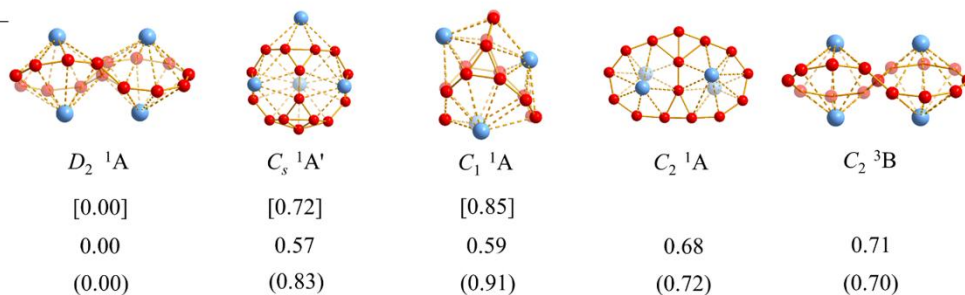
(3')  $\text{Ac}_2\text{B}_8$



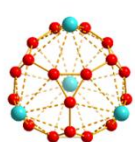
(4)  $\text{La}_4\text{B}_{15}^-$



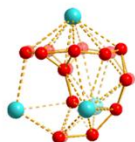
(4')  $\text{Ac}_4\text{B}_{15}^-$



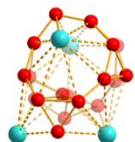
(5)  $\text{La}_4\text{B}_{18}$



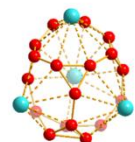
$C_{3v} \ ^1A_1$   
[0.00]  
0.00  
(0.00)



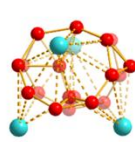
$C_s \ ^1A'$   
[0.07]  
0.09  
(0.21)



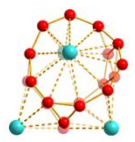
$C_1 \ ^1A$   
[0.81]  
0.71  
(0.85)



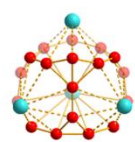
$C_1 \ ^1A$   
[0.86]  
0.75  
(0.98)



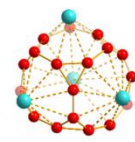
$C_s \ ^1A'$   
[1.02]  
0.79  
(1.03)



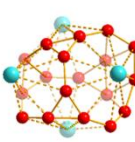
$C_1 \ ^1A$   
0.80  
(0.99)



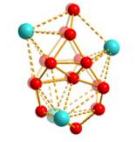
$C_s \ ^1A'$   
0.82  
(0.90)



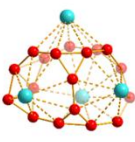
$C_1 \ ^1A$   
0.85  
(0.82)



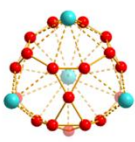
$C_1 \ ^1A$   
0.93  
(1.16)



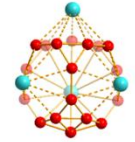
$C_s \ ^1A'$   
0.95  
(1.05)



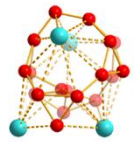
$C_1 \ ^1A$   
1.00  
(1.23)



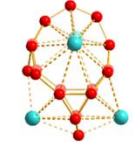
$C_s \ ^1A'$   
1.07  
(1.15)



$C_s \ ^1A'$   
1.07  
(1.26)

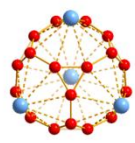


$C_1 \ ^3A$   
1.08  
(1.25)

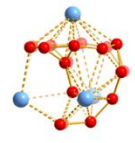


$C_s \ ^1A'$   
1.11  
(1.38)

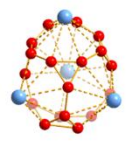
(5')  $\text{Ac}_4\text{B}_{18}$



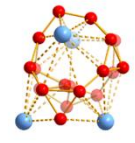
$C_3 \ ^1A$   
0.00  
(0.00)



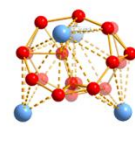
$C_s \ ^1A'$   
0.23  
(0.34)



$C_1 \ ^1A$   
0.93  
(1.07)

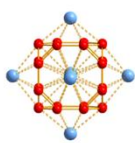


$C_1 \ ^1A$   
0.94  
(1.17)

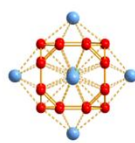


$C_s \ ^1A'$   
1.24  
(1.48)

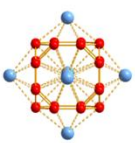
(6')  $\text{Ac}_7\text{B}_{24}^+$



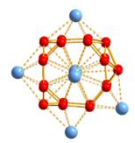
$O_h \ ^1A_{1g}$   
0.00  
(0.00)



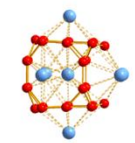
$C_i \ ^3A_u$   
1.06  
(1.13)



$C_1 \ ^5A_{1g}$   
2.18  
(2.29)

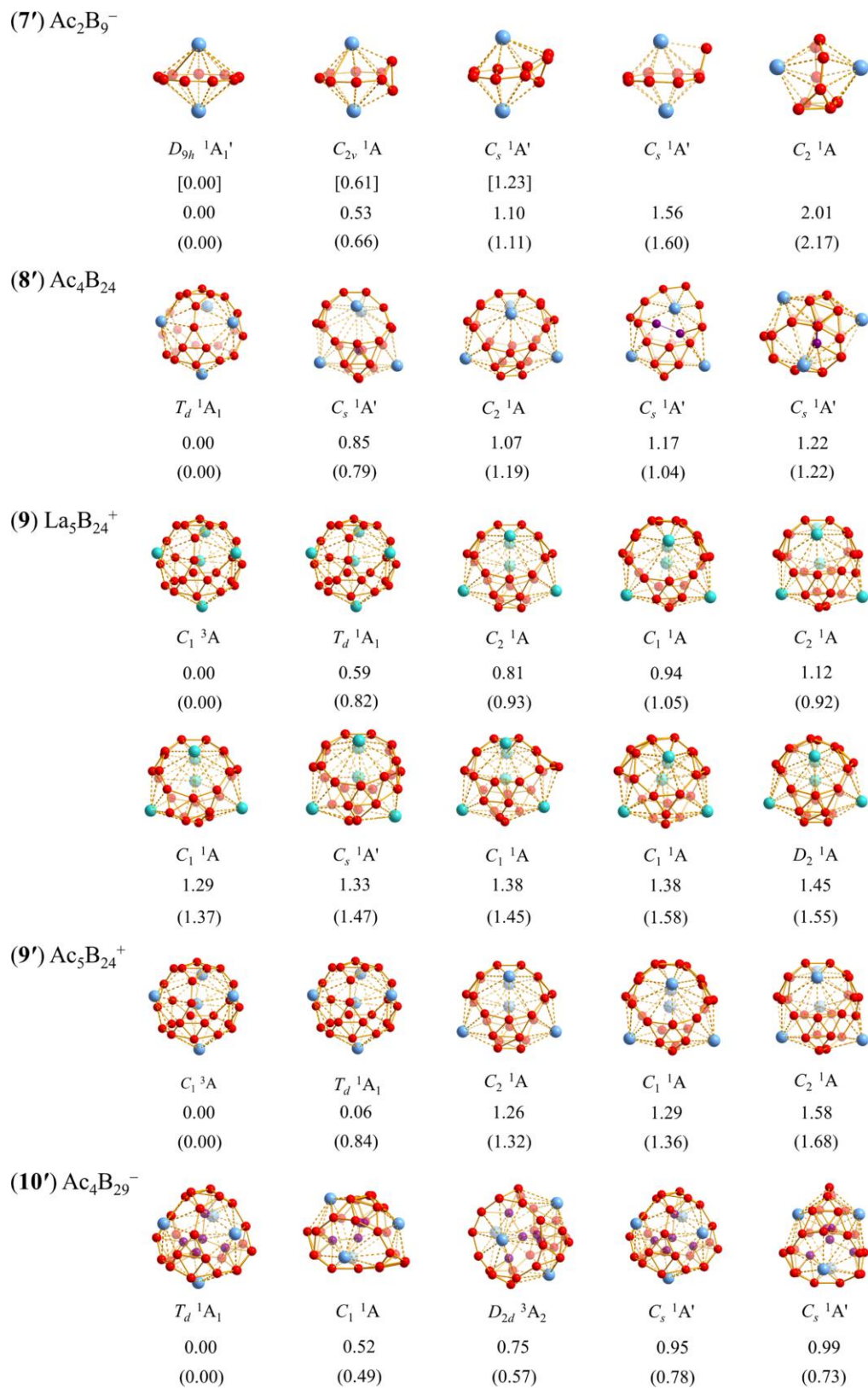


$C_s \ ^1A'$   
2.81  
(2.81)



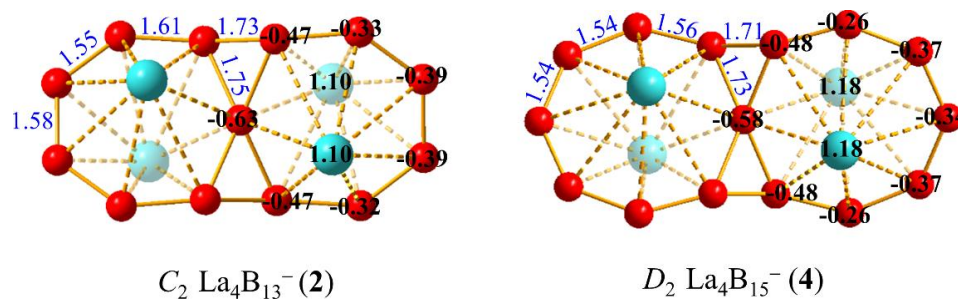
$C_{2v} \ ^1A_1$   
3.11  
(3.13)

**Fig. S3** Relative energies of low-lying isomers of  $D_{9h}$   $\text{Ac}_2\text{B}_9^-$  (**7'**),  $T_d$   $\text{Ac}_4\text{B}_{24}$  (**8'**),  $C_1$   $\text{M}_5\text{B}_{24}^+$  (**9/9'**), and  $T_d$   $\text{Ac}_4\text{B}_{29}^-$  (**10'**) (M = La, Ac) at CCSD(T) (square brackets), PBE0, and TPSSh (parentheses) levels in eV.

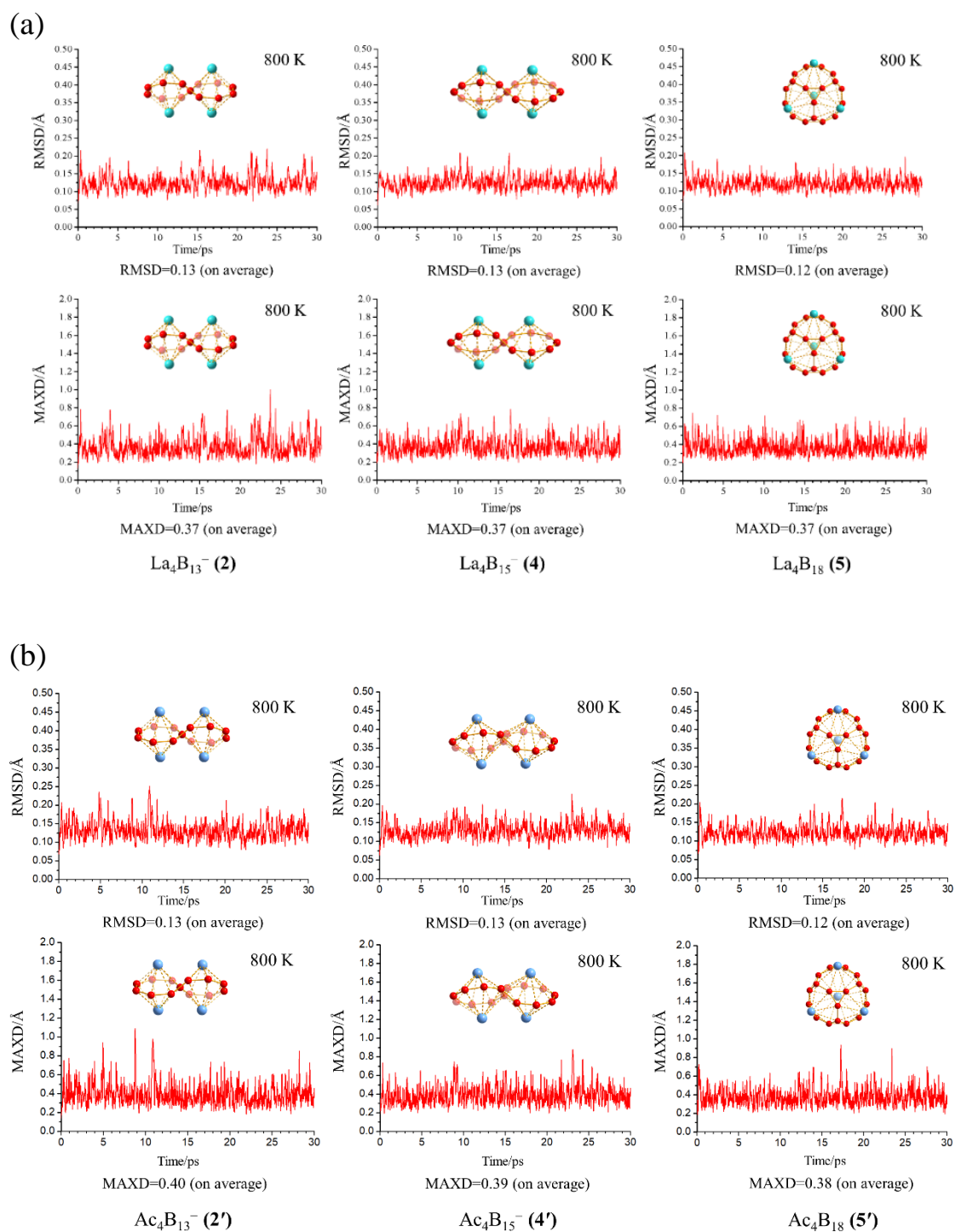




**Fig. S4** Geometry analysis and NBO analysis of bicyclic helical  $\text{La}_4\text{B}_{13}^-$  (**2**) and  $\text{La}_4\text{B}_{15}^-$  (**4**) at the PBE0 level. The B-B bond length is indicated in blue and the natural atomic charge is indicated in black.

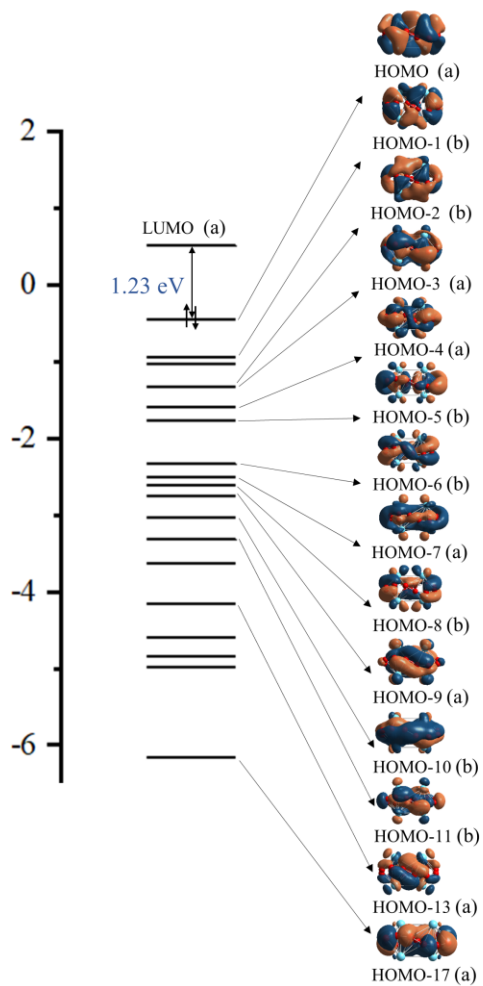


**Fig. S5** Born-Oppenheimer molecular dynamics simulations of  $M_4B_{13}^-$  (**2/2'**),  $M_4B_{15}^-$  (**4/4'**), and  $M_4B_{18}$  (**5/5'**) ( $M = La, Ac$ ) at 800 K. The root-mean-square-deviation (RMSD) and maximum bond length deviation (MAXD) values (on average) are indicated in Å.

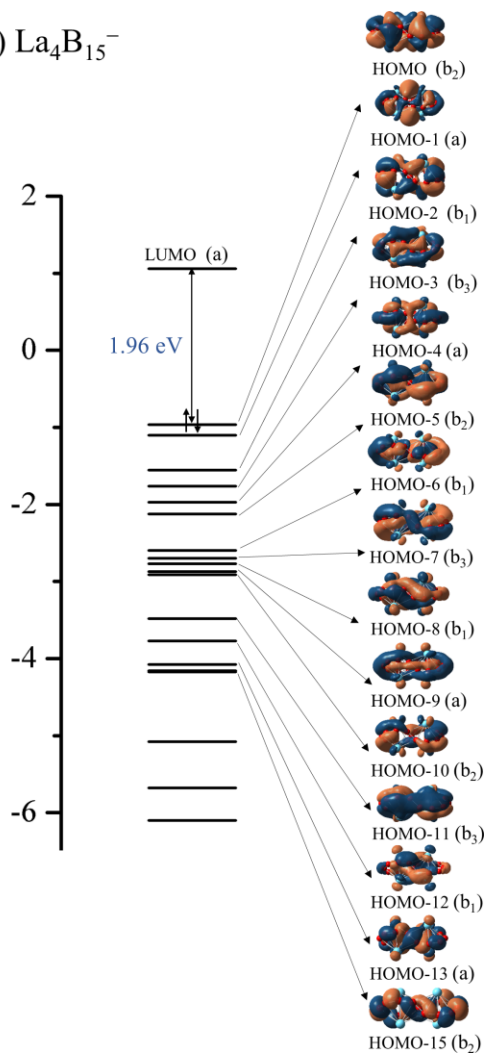


**Fig. S6** Canonical molecular orbitals (CMOs) of (a)  $\text{La}_4\text{B}_{13}^-$  (**2**), (b)  $\text{La}_4\text{B}_{15}^-$  (**4**), and (c)  $\text{La}_4\text{B}_{18}$  (**5**).

(a)  $\text{La}_4\text{B}_{13}^-$

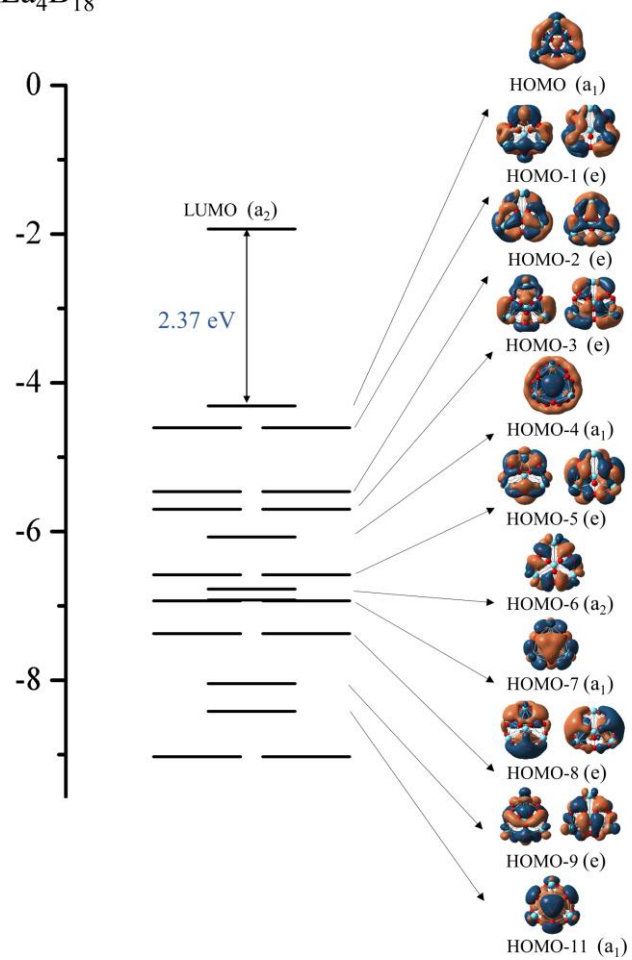


(b)  $\text{La}_4\text{B}_{15}^-$





(c)  $\text{La}_4\text{B}_{18}$



**Table S1** Optimized coordinates (x, y, z) of  $C_{2v}$   $Ac_2B_7^-$  (**1'**),  $C_2$   $La_4B_{13}^-$  (**2**)/ $Ac_4B_{13}^-$  (**2'**),  $D_{8h}$   $Ac_2B_8$  (**3'**),  $D_2$   $La_4B_{15}^-$  (**4**)/ $Ac_4B_{15}^-$  (**4'**),  $C_{3v}/C_3$   $La_4B_{18}$  (**5**)/ $Ac_4B_{18}$  (**5'**),  $O_h$   $Ac_7B_{24}^+$  (**6'**),  $D_{9h}$   $Ac_2B_9^-$  (**7'**),  $T_d$   $Ac_4B_{24}$  (**8'**),  $C_1$   $La_5B_{24}^+$  (**9**)/ $Ac_5B_{24}^+$  (**9'**), and  $T_d$   $Ac_4B_{29}^-$  (**10'**) at PBE0 level and 1D  $Ac_{10}B_{32}$  (**11'**), 2D  $Ac_3B_{10}$  (**12'**), and 3D  $AcB_6$  (**13'**) at PBE level.

$C_{2v}$   $Ac_2B_7^-$  (**1'**)

B	0.00000000	0.00000000	1.83250600
B	0.00000000	0.82123900	-1.64255100
B	0.00000000	1.78639500	-0.43470500
B	0.00000000	-1.78639500	-0.43470500
B	0.00000000	-1.41643600	1.14192200
B	0.00000000	1.41643600	1.14192200
B	0.00000000	-0.82123900	-1.64255100
Ac	1.99306600	0.00000000	0.00107200
Ac	-1.99306600	0.00000000	0.00107200

$C_2$   $La_4B_{13}^-$  (**2**)

B	0.00000000	3.57931400	-0.27819600
B	1.44471500	3.27564000	0.27733800
B	-1.12999600	2.57257100	-0.63454000
B	2.07188400	1.89844400	0.63452500
B	1.63180500	0.35173800	0.53783600
B	0.00000000	0.00000000	0.00032300
B	-1.35139300	0.97982700	-0.53745000
La	1.07511800	1.58077300	-1.80905700
La	-0.34525100	1.88063000	1.80908500
B	0.00000000	-3.57931400	-0.27819600
B	1.12999600	-2.57257100	-0.63454000
B	-2.07188400	-1.89844400	0.63452500
B	-1.63180500	-0.35173800	0.53783600
B	1.35139300	-0.97982700	-0.53745000
B	-1.44471500	-3.27564000	0.27733800
La	0.34525100	-1.88063000	1.80908500
La	-1.07511800	-1.58077300	-1.80905700

$C_2 \text{Ac}_4\text{B}_{13}^-$  (**2'**)

B	0.00000000	3.57513300	-0.26923100
B	1.45034600	3.26788900	0.26889500
B	-1.12842600	2.57191700	-0.63000600
B	2.07475600	1.89324300	0.63014800
B	1.63989000	0.34963400	0.52751000
B	0.00000000	0.00000000	0.00022700
B	-1.35718900	0.98463500	-0.52743700
B	0.00000000	-3.57513300	-0.26923100
B	1.12842600	-2.57191700	-0.63000600
B	-2.07475600	-1.89324300	0.63014800
B	-1.63989000	-0.34963400	0.52751000
B	1.35718900	-0.98463500	-0.52743700
B	-1.45034600	-3.26788900	0.26889500
Ac	-0.36544600	1.90584100	1.90404300
Ac	1.10723900	1.59351100	-1.90404300
Ac	-1.10723900	-1.59351100	-1.90404300
Ac	0.36544600	-1.90584100	1.90404300

 $D_{8h} \text{Ac}_2\text{B}_8$  (**3'**)

B	0.00000000	2.03032500	0.00000000
B	-1.43565600	1.43565600	0.00000000
B	1.43565600	1.43565600	0.00000000
B	-2.03032500	0.00000000	0.00000000
B	-1.43565600	-1.43565600	0.00000000
B	0.00000000	-2.03032500	0.00000000
B	1.43565600	-1.43565600	0.00000000
B	2.03032500	0.00000000	0.00000000
Ac	0.00000000	0.00000000	1.93885400
Ac	0.00000000	0.00000000	-1.93885400

$D_2 \text{La}_4\text{B}_{15}^-$  (4)

B	-1.50069700	0.56929900	-0.63502400
B	-1.89021800	0.74473900	-2.14033600
B	1.50069700	-0.56929900	-0.63502400
B	1.89021800	-0.74473900	-2.14033600
B	1.33622700	-0.50074400	-3.56125000
B	0.00000000	0.00000000	-4.14989400
B	-1.33622700	0.50074400	-3.56125000
B	1.50069700	0.56929900	0.63502400
B	0.00000000	0.00000000	0.00000000
B	1.89021800	0.74473900	2.14033600
B	-1.50069700	-0.56929900	0.63502400
B	-1.89021800	-0.74473900	2.14033600
B	-1.33622700	-0.50074400	3.56125000
B	0.00000000	0.00000000	4.14989400
B	1.33622700	0.50074400	3.56125000
La	-0.66219000	1.69877700	1.96403300
La	0.66219000	-1.69877700	1.96403300
La	-0.66219000	-1.69877700	-1.96403300
La	0.66219000	1.69877700	-1.96403300

$D_2 \text{Ac}_4\text{B}_{15}^-$  (4')

B	-1.49909300	0.56992700	-0.64381500
B	-1.89482400	0.73370600	-2.15224000
B	1.49909300	-0.56992700	-0.64381500
B	1.89482400	-0.73370600	-2.15224000
B	1.34366800	-0.49164000	-3.57740800
B	0.00000000	0.00000000	-4.16592700
B	-1.34366800	0.49164000	-3.57740800
B	1.49909300	0.56992700	0.64381500
B	0.00000000	0.00000000	0.00000000
B	1.89482400	0.73370600	2.15224000
B	-1.49909300	-0.56992700	0.64381500
B	-1.89482400	-0.73370600	2.15224000
B	-1.34366800	-0.49164000	3.57740800
B	0.00000000	0.00000000	4.16592700
B	1.34366800	0.49164000	3.57740800
Ac	0.68597600	1.76900000	-1.99290000
Ac	-0.68597600	1.76900000	1.99290000
Ac	-0.68597600	-1.76900000	-1.99290000
Ac	0.68597600	-1.76900000	1.99290000

$C_{3v} \text{La}_4\text{B}_{18} (5)$ 

B	-0.81707700	-0.47174000	-1.33615400
B	0.00000000	0.94347900	-1.33615400
B	0.00000000	2.41248300	-0.49245800
B	-0.85327800	2.66607700	0.87128700
B	-2.07402800	2.07088900	1.69302900
B	-2.08927100	-1.20624100	-0.49245800
B	2.08927100	-1.20624100	-0.49245800
B	2.07402800	2.07088900	1.69302900
B	0.85327800	2.66607700	0.87128700
B	0.81707700	-0.47174000	-1.33615400
B	-2.73552900	-0.59407900	0.87128700
B	-2.83045600	0.76071600	1.69302900
B	-0.75642800	-2.83160500	1.69302900
B	-1.88225200	-2.07199900	0.87128700
B	0.75642800	-2.83160500	1.69302900
B	1.88225200	-2.07199900	0.87128700
B	2.73552900	-0.59407900	0.87128700
B	2.83045600	0.76071600	1.69302900
La	0.00000000	0.00000000	1.75860000
La	-2.58473900	1.49230000	-0.87567500
La	2.58473900	1.49230000	-0.87567500
La	0.00000000	-2.98459900	-0.87567500



$C_3 \text{Ac}_4\text{B}_{18} (5')$ 

B	-0.81798000	-0.47237700	-1.27427900
B	-0.00010100	0.94458000	-1.27427900
B	0.00000000	2.41907700	-0.42539600
B	-0.85622100	2.67188800	0.93316100
B	-2.09427500	2.08235800	1.74842100
B	-2.09498200	-1.20953800	-0.42539600
B	2.09498200	-1.20953800	-0.42539600
B	2.09368800	2.08183600	1.74963800
B	0.85601200	2.67196300	0.93388000
B	0.81808000	-0.47220300	-1.27427900
B	-2.74199400	-0.59465300	0.93388000
B	-2.84976700	0.77226900	1.74963800
B	-0.75623800	-2.85487400	1.74842100
B	-1.88581200	-2.07745300	0.93316100
B	0.75607900	-2.85410500	1.74963800
B	1.88598100	-2.07731000	0.93388000
B	2.74203300	-0.59443500	0.93316100
B	2.85051200	0.77251600	1.74842100
Ac	0.00000000	0.00000000	1.96249800
Ac	-2.63942300	1.52236900	-0.86008900
Ac	0.00130100	-3.04699200	-0.86008900
Ac	2.63812200	1.52462300	-0.86008900

$O_h \text{Ac}_7\text{B}_{24}^+ (6')$ 

B	0.84799800	2.01422200	2.01422200
B	2.01422200	2.01422200	0.84799800
B	2.01422200	2.01422200	-0.84799800
B	0.84799800	2.01422200	-2.01422200
B	-0.84799800	2.01422200	-2.01422200
B	-0.84799800	2.01422200	2.01422200
B	2.01422200	-0.84799800	2.01422200
B	2.01422200	-0.84799800	-2.01422200
B	2.01422200	0.84799800	-2.01422200
B	2.01422200	0.84799800	2.01422200
B	-2.01422200	2.01422200	0.84799800
B	-2.01422200	2.01422200	-0.84799800
B	-2.01422200	0.84799800	-2.01422200
B	-2.01422200	-0.84799800	-2.01422200
B	-2.01422200	-2.01422200	-0.84799800
B	-2.01422200	-2.01422200	0.84799800
B	-2.01422200	-0.84799800	2.01422200
B	-2.01422200	0.84799800	2.01422200
B	0.84799800	-2.01422200	-2.01422200
B	-0.84799800	-2.01422200	-2.01422200
B	-0.84799800	-2.01422200	2.01422200
B	0.84799800	-2.01422200	2.01422200
B	2.01422200	-2.01422200	0.84799800
B	2.01422200	-2.01422200	-0.84799800
Ac	0.00000000	3.75081700	0.00000000
Ac	-3.75081700	0.00000000	0.00000000
Ac	0.00000000	0.00000000	3.75081700
Ac	0.00000000	0.00000000	0.00000000
Ac	0.00000000	0.00000000	-3.75081700
Ac	3.75081700	0.00000000	0.00000000
Ac	0.00000000	-3.75081700	0.00000000

$D_{9h} \text{Ac}_2\text{B}_9^- (7')$

B	0.00000000	2.25385200	0.00000000
B	1.44874800	1.72655100	0.00000000
B	2.21961100	0.39137700	0.00000000
B	1.95189300	-1.12692600	0.00000000
B	0.77086300	-2.11792800	0.00000000
B	-0.77086300	-2.11792800	0.00000000
B	-1.95189300	-1.12692600	0.00000000
B	-2.21961100	0.39137700	0.00000000
B	-1.44874800	1.72655100	0.00000000
Ac	0.00000000	0.00000000	1.80853500
Ac	0.00000000	0.00000000	-1.80853500

$T_d \text{Ac}_4\text{B}_{24} \text{(8')}$ 

B	0.83696700	-2.00045600	2.00045600
B	-0.55744000	0.55744000	2.79213700
B	2.00045600	-2.00045600	0.83696700
B	-0.83696700	2.00045600	2.00045600
B	-0.55744000	2.79213700	0.55744000
B	0.55744000	0.55744000	-2.79213700
B	2.00045600	0.83696700	-2.00045600
B	0.55744000	2.79213700	-0.55744000
B	0.55744000	-2.79213700	0.55744000
B	-0.55744000	-0.55744000	-2.79213700
B	-2.79213700	0.55744000	0.55744000
B	-2.79213700	-0.55744000	-0.55744000
B	-2.00045600	2.00045600	0.83696700
B	2.79213700	-0.55744000	0.55744000
B	2.00045600	2.00045600	-0.83696700
B	0.55744000	-0.55744000	2.79213700
B	2.00045600	-0.83696700	2.00045600
B	-0.55744000	-2.79213700	-0.55744000
B	2.79213700	0.55744000	-0.55744000
B	0.83696700	2.00045600	-2.00045600
B	-0.83696700	-2.00045600	-2.00045600
B	-2.00045600	-0.83696700	-2.00045600
B	-2.00045600	-2.00045600	-0.83696700
B	-2.00045600	0.83696700	2.00045600
Ac	1.85877900	1.85877900	1.85877900
Ac	-1.85877900	-1.85877900	1.85877900
Ac	-1.85877900	1.85877900	-1.85877900
Ac	1.85877900	-1.85877900	-1.85877900

$C_1 \text{La}_5\text{B}_{24}^+$  (9)

B	-2.71437600	0.65169600	0.85398700
B	-0.98165500	-1.20101200	2.47091800
B	-2.74786500	0.54284000	-0.83758400
B	0.41074800	-2.00040500	2.08629700
B	1.57664100	-2.32656200	0.91618800
B	1.64515200	0.22152200	-2.41572100
B	0.40147100	-0.85943000	-2.72495300
B	1.54745100	-2.43336700	-0.66130900
B	-2.18399500	1.91150400	-0.08788500
B	1.71082200	1.66117100	-1.73379300
B	1.72678100	0.52944100	2.30698000
B	1.76382600	1.86967500	1.44689600
B	1.85701200	-1.09383800	2.01348300
B	-2.34394600	-0.93001200	-1.49295200
B	0.34484000	-2.25975300	-1.82380000
B	-2.29209000	-0.72464900	1.68297200
B	-2.79000200	-0.86779200	0.10588700
B	-0.83569800	2.77443100	-0.16271300
B	-1.06118200	-1.51034700	-2.25510500
B	1.78880700	-1.34854100	-1.91529500
B	0.57874100	2.66168300	-1.02278700
B	1.96385700	2.17920500	-0.17549300
B	0.60717400	2.77578400	0.65213500
B	0.49407700	-0.49960300	2.79861400
La	0.01366100	-0.00759600	0.00043400
La	3.31892000	-0.13706600	-0.04651100
La	-1.25648900	-3.05449100	0.21699300
La	-1.01168600	1.78760200	2.58125100
La	-1.10533400	1.43579300	-2.75435700

$C_1 \text{Ac}_5\text{B}_{24}^+(9')$ 

B	-2.44276300	-0.41195200	-1.60675900
B	-1.58563900	0.67396300	2.37397300
B	-2.09350000	-1.87538900	0.83050200
B	-2.09051900	-1.86548400	-0.86177000
B	-1.57442100	0.70264600	-2.37271600
B	0.05166300	0.84753900	-2.77864000
B	-0.75047400	2.04947000	1.98555900
B	-2.45117600	-0.43094300	1.59117100
B	-0.95808200	-2.74868600	-0.01854800
B	-2.87152800	-0.62050500	-0.00985300
B	2.38996400	-0.67560900	-1.59764600
B	1.87851800	-2.08268800	-0.85418800
B	0.15566500	2.85560700	0.81065400
B	-0.74230900	2.07382900	-1.96336700
B	0.97204800	1.98086700	-1.96019300
B	0.96337800	1.95593900	1.98938400
B	0.03931400	0.81195800	2.78739700
B	1.64076800	0.49633300	2.38033200
B	0.65218600	-2.83589900	-0.01644900
B	2.38393300	-0.69576400	1.60050400
B	1.87363900	-2.09247900	0.83672200
B	0.15953400	2.86679900	-0.77558200
B	2.78732700	-0.92992100	0.00100900
B	1.65110400	0.52629400	-2.36641200
Ac	0.00107700	0.01112000	-0.00027600
Ac	-2.67350100	2.10316400	0.00732400
Ac	-0.11443100	-1.99036300	2.73037500
Ac	2.88718800	1.79967100	0.01713900
Ac	-0.10250400	-1.95594700	-2.75484600



$T_d \text{Ac}_4\text{B}_{29}^- (10')$ 

B	-0.89006500	-2.18991700	-2.18991700
B	0.64678100	0.64678100	-2.80385900
B	-2.18991700	-2.18991700	-0.89006500
B	0.89006500	2.18991700	-2.18991700
B	0.64678100	2.80385900	-0.64678100
B	-0.64678100	0.64678100	2.80385900
B	-2.18991700	0.89006500	2.18991700
B	-0.64678100	2.80385900	0.64678100
B	-0.64678100	-2.80385900	-0.64678100
B	0.64678100	-0.64678100	2.80385900
B	2.80385900	0.64678100	-0.64678100
B	2.80385900	-0.64678100	0.64678100
B	2.18991700	2.18991700	-0.89006500
B	-2.80385900	-0.64678100	-0.64678100
B	-2.18991700	2.18991700	0.89006500
B	-0.64678100	-0.64678100	-2.80385900
B	-2.18991700	-0.89006500	-2.18991700
B	0.64678100	-2.80385900	0.64678100
B	-2.80385900	0.64678100	0.64678100
B	-0.89006500	2.18991700	2.18991700
B	0.89006500	-2.18991700	2.18991700
B	2.18991700	-0.89006500	2.18991700
B	2.18991700	-2.18991700	0.89006500
B	2.18991700	0.89006500	-2.18991700
B	0.96009800	-0.96009800	0.96009800
B	-0.96009800	0.96009800	0.96009800
B	-0.96009800	-0.96009800	-0.96009800
B	0.96009800	0.96009800	-0.96009800
B	0.00000000	0.00000000	0.00000000
Ac	1.73449400	1.73449400	1.73449400
Ac	-1.73449400	1.73449400	-1.73449400
Ac	-1.73449400	-1.73449400	1.73449400
Ac	1.73449400	-1.73449400	-1.73449400

1D Ac<sub>10</sub>B<sub>32</sub> (11')

B	0.3477020	0.6409886	0.6181548
B	0.8494163	0.6414765	0.6186604
B	0.3477266	0.6409838	0.4297470
B	0.8494333	0.6414808	0.4292516
B	0.1616680	0.6414840	0.4292470
B	0.6633540	0.6409820	0.4297501
B	0.1616642	0.6414828	0.6186662
B	0.6633588	0.6409837	0.6181505
B	0.0055566	0.6543564	0.5683319
B	0.5055177	0.6564455	0.5704792
B	0.0055615	0.6543474	0.4795885
B	0.5055223	0.6564560	0.4774107
B	0.0055650	0.5913266	0.4162447
B	0.5055280	0.5934303	0.4142494
B	0.0055667	0.5022844	0.4162601
B	0.5055303	0.5001164	0.4142203
B	0.0055643	0.4392375	0.4795508
B	0.5055276	0.4372143	0.4775386
B	0.0055594	0.4392303	0.5683725
B	0.5055231	0.4372276	0.5703536
B	0.0055558	0.5022997	0.6316553
B	0.5055177	0.5000769	0.6337213
B	0.0055541	0.5913156	0.6316696
B	0.5055154	0.5934751	0.6336917
B	0.3477551	0.4525877	0.4297451
B	0.8494254	0.4521102	0.4292371
B	0.1616834	0.4521089	0.4292356
B	0.6633331	0.4525875	0.4297453
B	0.1616792	0.4521139	0.6186802
B	0.6633370	0.4525899	0.6181575
B	0.3477311	0.4525870	0.6181587
B	0.8494091	0.4521183	0.6186776
Ac	0.2388177	0.5467906	0.5239506
Ac	0.7723804	0.5467881	0.5239477
Ac	0.2575022	0.7321750	0.5239478
Ac	0.7535619	0.7321548	0.5239499

Ac	0.2573273	0.3614945	0.5239500
Ac	0.7537482	0.3615133	0.5239526
Ac	0.2575167	0.5467796	0.3385873
Ac	0.7535718	0.5467806	0.3386055
Ac	0.2575661	0.5467835	0.7093229
Ac	0.7534859	0.5467843	0.7093028

2D Ac<sub>10</sub>B<sub>32</sub> (12')

B	0.6877102	0.0042564	0.6027397
B	0.9875225	0.0042604	0.5430821
B	0.2873359	0.0042566	0.6027396
B	0.9875229	0.3040693	0.6027397
B	0.9875234	0.3040788	0.4030192
B	0.9875232	0.7044676	0.4030189
B	0.9875227	0.7044436	0.6027396
B	0.6877179	0.0042726	0.4030190
B	0.2873292	0.0042728	0.4030191
B	0.9875227	0.0042680	0.4626760
Ac	0.4875189	0.5042605	0.5028782
Ac	0.4875208	0.5042748	0.3175972
Ac	0.4875199	0.5042486	0.6881617

3D AcB<sub>6</sub> (13')

B	0.7075093	0.9819103	0.9987204
B	0.0064796	0.9819103	0.6997495
B	0.0064796	0.9819103	0.2976898
B	0.3054497	0.9819103	0.9987204
B	0.0064796	0.2808798	0.9987203
B	0.0064796	0.6829395	0.9987203
Ac	0.5064825	0.4819193	0.4987292