

Supporting Information

Transition from exohedral to endohedral geometries of anionic and neutral B_4Si_n ($n = 4-15$) clusters: quantum chemical calculations

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Theoretical method

CALYPSO is based on the generalization of particle swarm optimization (PSO). A large number of low-energy initial structures are randomly generated with the constraint of symmetries. The success of CALYPSO is due to the integration of several major techniques including structural evolution through PSO algorithm, symmetry constraint during structure generation, the Metropolis criterion, atom-centered symmetrical function, and bond characterization matrix (BCM), which can enhance the capability of CALYPSO in dealing with more complex systems and also reduce searching space, enhance the structural diversity, and eliminate similar structures on the potential energy surfaces to enhance searching efficiency. Here, structure predictions of anionic and neutral B_4Si_n ($n = 4-15$) clusters are carried out. Cluster structures are ordered by generations in the particle swarm optimization method, in which each generation includes 100 structures, 70% of which are generated by the particle swarm optimization algorithm at the HSE06/6-31+G(d) level, while the others are generated randomly. Subsequently, we have picked out 40 generations to achieve convergence around the lowest minima of the potential energy surfaces. The searches can obtain a large database for low-energy anionic and neutral B_4Si_n ($n = 4-15$) clusters. These low-energy structures within 2 eV of the global minimum structure are reoptimized with subsequent geometrical optimizations and frequency analyses at the HSE06/def2-TZVP level.

Table S1. Cartesian coordinates for stable isomers of $B_4Si_{4-15}^-$ clusters.

$B_4Si_4^-$							
4A				4B			
	X	Y	Z		X	Y	Z
Si	-0.81302827	-1.54426951	0.00000000	B	0.00003000	-0.01580300	-0.90401600
Si	0.81302827	1.54426951	0.00000000	B	-0.90072700	1.37468100	-0.53211400
Si	-2.45610215	0.43485217	0.00000000	B	0.90030400	1.37494100	-0.53269800
Si	2.45610215	-0.43485217	0.00000000	Si	0.00007100	-1.79603800	-0.04498100
B	-0.69869430	0.37665783	-0.94439618	Si	0.00025600	0.46668500	1.27608600
B	-0.69869430	0.37665783	0.94439618	Si	1.95060400	-0.30396100	-0.21077000
B	0.69869430	-0.37665783	-0.94439618	Si	-1.95065500	-0.30420700	-0.21063800
B	0.69869430	-0.37665783	0.94439618	B	-0.00037800	2.69124000	-0.29832500
4C				4D			
	X	Y	Z		X	Y	Z
B	0.47413100	0.00497500	1.04883300	Si	-0.03944800	0.00164500	1.21312500
B	-0.96364900	0.80426600	0.85512600	Si	-1.02637300	1.84490000	-0.16275900
B	-0.94257500	-0.83272900	0.84882200	Si	2.42998300	0.00020000	-0.07069200
Si	0.46627300	1.92408700	0.11204600	Si	-1.02764700	-1.84439600	-0.16172600
Si	0.51485600	-1.91600600	0.11026500	B	-0.57524800	-0.00115500	-0.97957100
Si	-2.27702400	-0.01939900	-0.49816100	B	-1.90679800	0.00113300	-0.04762900
Si	1.88902500	0.02138100	-0.47345500	B	0.77003100	0.89166400	-0.63443200
B	-0.22867100	-0.00468800	-0.65472900	B	0.76977400	-0.89821800	-0.62862100
$B_4Si_5^-$							
5A				5B			
	X	Y	Z		X	Y	Z
B	0.46111300	-0.01195400	0.86027000	Si	1.52037300	-0.49670700	1.27274400
B	-1.11514000	0.16555600	0.23876000	Si	-1.02520000	1.94020700	0.08108200
B	-0.33675900	-1.39241700	0.26960300	Si	2.56736100	0.36021800	-0.66332300
Si	2.19728400	0.76642700	0.25744200	Si	-0.83779700	-1.87075500	-0.39756500
Si	0.46840700	-0.08449900	-1.38029300	Si	-0.67311100	0.16633100	-1.00212800
Si	1.64695500	-1.61908700	0.29341900	Si	-0.34504200	-0.06108600	0.77115200
Si	-0.02434500	1.87362700	0.19176500	Si	0.68779800	1.00932700	-0.30610600
B	-1.93609800	-1.35836000	0.15192000	B	0.74226400	-0.67296100	-0.71184300
Si	-3.24298400	-0.00890500	0.09461200	B	-2.37184700	-0.09068100	0.15310600
5C				5D			
	X	Y	Z		X	Y	Z
B	0.75392200	0.25456600	-0.99982700	B	0.00067700	-0.12780300	-0.53979400
B	-0.82972200	-0.20497800	-0.87767000	B	-0.84269600	0.12769700	1.06332400
B	-0.41340100	1.35040300	-0.37705700	B	0.83897700	0.13537600	1.06000800
Si	0.42878700	-1.78829800	-0.60025900	Si	1.57806700	-1.54272100	-0.14355700
Si	1.37947000	1.82623500	0.26442800	Si	2.01350000	0.80810600	-0.48474100
Si	-2.38836500	0.96658900	-0.28038300	Si	-2.03251700	0.79087400	-0.46173100
Si	2.24153900	-0.44852600	0.24669000	Si	-0.00494200	1.92065800	0.32591400
B	0.20253600	-0.02343100	0.72305600	Si	-1.55392300	-1.55955500	-0.17201900
Si	-1.55905100	-1.04762900	0.91648700	B	0.00252200	-1.30388400	1.03763900

$B_4Si_6^-$

6A				6B			
	X	Y	Z		X	Y	Z
B	0.43526800	0.00030400	-0.52820900	B	-0.38140500	-0.17775200	-0.70940700
B	1.08269600	-0.00123400	1.19902700	B	0.85596100	0.45022000	0.43284700
B	-0.38802000	-0.83109600	1.02577100	B	0.24951100	-1.21961500	0.61057400
Si	-2.30232800	0.00104800	0.94020900	Si	-2.29963600	0.49172400	-0.75997900
Si	-1.23770100	-1.25290300	-0.97361800	Si	-1.12140700	0.36365400	1.43371200
Si	2.49712000	-0.00021200	-0.25572900	Si	-1.66924600	-1.68298900	0.12917700
Si	1.00656600	-1.95952300	0.14584800	Si	-0.34596600	1.91891300	-0.35054400
Si	1.00683400	1.95926500	0.14670600	B	1.80587800	-0.98455900	0.88462600
B	-0.38693000	0.83163400	1.02663200	Si	2.95859600	0.43831000	0.35949300
Si	-1.23585300	1.25246400	-0.97599500	Si	1.57410700	-0.83971600	-1.24708800
6C				6D			
	X	Y	Z		X	Y	Z
B	0.70903600	-0.46869700	0.83478600	B	0.86318900	0.21785300	-0.92937400
B	-0.68577200	0.46482500	0.81538900	B	-0.78411700	0.46552000	-0.60392000
B	-0.70918300	-0.47073900	-0.83796000	B	-0.15443700	-1.14625900	-0.86483900
Si	0.90530000	1.76074800	0.90661400	Si	2.53966900	0.67900500	0.06430700
Si	0.88946500	-1.75882000	-0.91548200	Si	0.65153300	-0.32010000	1.24606900
Si	-2.49589200	-0.00221600	0.00490600	Si	1.79250800	-1.59493800	-0.65340300
Si	2.49615300	-0.00365000	-0.00679500	Si	0.43994400	1.96899000	0.03316600
B	0.68620500	0.46671500	-0.81816000	B	-1.74518000	-0.94294400	-0.96360200
Si	-0.90353800	1.76345700	-0.90450700	Si	-2.87646800	0.56040700	-0.63190700
Si	-0.89159100	-1.75669800	0.91738700	Si	-1.89699200	-0.79128300	1.14238800

 $B_4Si_7^-$

7A				7B			
	X	Y	Z		X	Y	Z
B	-0.74027100	0.44498200	0.61312800	B	0.94830000	-0.63144000	0.63530900
B	-0.71754900	-0.74108400	-0.91980200	B	-0.94856200	0.61913500	0.64191100
B	0.61728500	-1.15275200	0.17363000	B	-0.76714700	-0.34614500	-1.28859000
Si	2.35954800	-0.09745100	-0.19179400	Si	1.00716400	1.56277600	0.73733500
Si	0.85040300	-0.03140600	1.95910100	Si	0.68597800	-1.78822800	-1.11093900
Si	-2.56982800	-0.28548200	-0.26982000	Si	-2.52097700	0.09202200	-0.56352300
Si	-1.10904800	-1.46192100	1.28441600	Si	2.51944400	-0.08956900	-0.56619400
Si	-1.21016800	1.61462600	-1.00669000	B	0.76607100	0.36095100	-1.28816600
B	0.54542100	0.46716100	-1.00264200	Si	-0.68837000	1.80186600	-1.09039400
Si	0.71531900	2.00107200	0.43206900	Si	-1.00665600	-1.57030500	0.72781600
Si	1.06917300	-1.38883300	-1.80167900	Si	0.00389600	-0.00945400	2.33001900
7C				7D			
	X	Y	Z		X	Y	Z
Si	-2.16658700	-1.85748100	-0.37525100	B	0.35130900	0.94254800	-0.12425700
Si	1.37793400	-1.91627900	-0.29859700	B	0.35118400	-0.94991200	-0.05886100
Si	0.92674100	0.00226300	1.34662900	B	-0.79214500	0.03354900	0.94387400
Si	2.90120200	-0.00402100	-0.12715400	Si	2.40184600	1.30656800	-0.06516500
B	-0.37671000	-0.86344700	-0.59968400	Si	2.40569300	-1.30524300	0.02074000
B	-0.37462600	0.86541200	-0.59860400	Si	1.17696400	0.05758200	1.67734100
B	1.05140200	-0.00160500	-0.91299400	Si	-2.72882500	0.04050300	1.13985300
B	-1.84763100	0.00304200	-0.93976300	Si	-1.59377900	1.55023800	-0.40845300
Si	-2.16084100	1.86292800	-0.36555200	Si	-0.50846100	-0.06845600	-1.91668300
Si	-1.71071900	-0.00200300	1.21729000	Si	-1.59390200	-1.57536500	-0.29450100
Si	1.38497200	1.91337800	-0.30770600	B	1.32295600	-0.04250000	-1.18952400



8A			8B				
	X	Y	Z		X	Y	Z
B	0.91868900	0.05064700	-0.49094600	B	0.08235300	-1.42174400	0.39245300
B	0.85437700	-0.06279000	1.35559200	B	1.10690700	0.36288200	0.64394900
B	-0.11882200	-1.20376400	0.53240600	B	-0.43843500	-0.02464600	1.34368000
Si	-2.05994800	-1.26921300	-0.02869900	Si	-2.08129000	1.08206300	1.21989400
Si	-0.08031900	-1.45168200	-1.61315900	Si	-1.93704100	-1.24218600	0.24594700
Si	2.69824600	0.40528700	0.67170300	Si	1.97865500	-1.29789800	-0.31193800
Si	1.73863900	-1.79047300	0.07008300	Si	1.16305400	-1.09477400	2.08733800
Si	1.13914400	2.13077500	-0.40967600	Si	1.54469600	2.37006400	0.19305200
B	-0.26733900	1.09079200	0.56946700	B	-0.18799900	1.45901100	0.31303500
Si	-0.55649700	0.95711600	-1.67427300	Si	0.90338900	0.79218800	-1.52252500
Si	-1.10563800	-0.11957400	2.07464300	Si	-0.25586500	-1.44726100	-1.67416500
Si	-2.26895000	1.18244800	0.20705100	Si	-1.51660800	0.70369500	-1.19943000
8C			8D				
	X	Y	Z		X	Y	Z
B	0.09661100	0.90985400	0.45425900	B	0.39238700	-0.52562900	-1.29241400
B	-1.06230200	0.00293200	-1.53952700	B	-1.00530800	-1.22163400	-0.69725000
B	0.09726400	-0.91062200	0.45085500	B	-0.68952900	0.41975600	0.11151500
Si	2.01520900	-1.34009000	-0.31396900	Si	0.67513200	-2.40059000	0.00570100
Si	1.45544000	-0.00376300	1.84762600	Si	1.95313500	1.32359600	0.16179400
Si	-1.97627700	1.31967300	0.12353000	Si	-2.67883800	-0.40462400	-0.13339700
Si	-0.99540700	-0.00419000	1.99359100	Si	2.30584900	-0.83789300	-0.98655700
Si	-0.21614500	1.89936400	-1.43384300	B	0.90265200	-0.42255100	0.55115100
B	0.57493500	0.00175700	-1.00547800	Si	-0.83773200	-1.15034700	1.63906700
Si	2.01420900	1.34196300	-0.30948500	Si	-1.20888100	0.62685800	-1.88087700
Si	-0.21603400	-1.89399100	-1.44045600	Si	-0.28565900	2.39348600	-0.21944300
Si	-1.97617600	-1.32036600	0.11868100	Si	0.21977900	1.07453500	1.88764000



9A				9B			
	X	Y	Z		X	Y	Z
B	-0.58823100	0.63337300	0.69523000	B	0.18036000	-0.90426900	0.92939400
B	-0.57207900	0.31045000	-1.02394200	B	1.16661800	-0.00014800	-0.16442100
B	-0.29784400	-1.01430100	0.12179000	B	0.18085500	0.90459400	0.92922900
Si	1.69880000	-1.77461600	0.36852900	Si	-0.11011000	-1.33621400	-1.26232900
Si	0.34564200	-0.58321100	2.08388800	Si	-1.27852900	0.00037500	2.15197600
Si	-2.44352700	1.05132000	-0.34488500	Si	1.83102300	1.93094900	0.23187700
Si	-2.03881200	-0.84616700	1.36040100	Si	-1.61491000	-1.93345500	0.58224500
Si	-0.30618200	2.40310700	-0.47815300	B	-2.05410500	0.00106300	0.17085300
B	0.98030000	0.96919900	-1.16085300	Si	-0.10888600	1.33394000	-1.26383300
Si	1.31829600	1.48100100	1.09716300	Si	3.27515500	-0.00053100	-0.05935200
Si	0.75437000	-1.08437000	-1.77016500	Si	1.82956500	-1.93150400	0.23430200
Si	2.76490600	0.33051500	-0.60416400	Si	-2.02243200	0.00132300	-1.86567400
Si	-1.92283100	-1.29854900	-1.22412300	Si	-1.61292300	1.93467400	0.58469600
9C				9D			
	X	Y	Z		X	Y	Z
B	-0.85610800	0.51358000	0.70291900	B	0.78353600	0.17587500	-0.45468500
B	-0.51382400	-1.03884200	-0.02143200	B	0.32258600	0.47836600	1.22866700
B	0.95452300	-0.53504300	-1.19109700	B	-0.03712700	-1.11501900	0.55428100
Si	1.33432100	1.50960600	-1.23660300	Si	-1.96538100	-1.59037900	-0.18897200
Si	0.88222100	1.64671100	1.33485300	Si	0.20759800	-1.46432800	-1.52432100
Si	-2.10943700	-1.01118800	1.38246200	Si	2.22582700	1.26576300	0.70888700
Si	0.28481000	-0.67960700	1.94183500	Si	1.81801800	-1.22865100	1.25602400
Si	-2.51628400	0.45098300	-0.59967500	Si	0.24142600	2.23642800	-0.31443700
B	-0.49615100	0.31119700	-1.14331300	B	-1.13142900	1.31020000	0.76733700
Si	-0.86646500	2.28304300	-0.43163600	Si	-0.94823600	0.66784500	-1.75677500
Si	-0.40650700	-1.70892700	-2.03215300	Si	-1.49305500	-0.39399300	1.93157800
Si	1.23232000	-2.18750000	0.02780000	Si	-2.83865200	0.72253400	-0.01216200
Si	2.49057700	-0.03558300	0.20344700	Si	2.77475300	-0.51858400	-0.84825200



10A				10B			
	X	Y	Z		X	Y	Z
B	-0.19949500	0.85970300	-0.80317200	B	0.47914100	-0.91201100	0.64130800
B	-0.19636400	-0.86089800	-0.79190600	B	0.53676900	0.82850900	0.25240700
B	-1.06909700	0.00364700	0.55013900	B	-0.81739400	0.89437600	-1.05611100
Si	1.61090100	-1.89913000	-0.12367900	Si	-1.55333800	-0.95698000	-1.65696400
Si	3.35113000	0.00103500	-0.17078900	Si	-1.61068500	-1.45117800	1.04500400
Si	1.60585700	1.89944300	-0.12436800	Si	2.24105500	0.00700300	1.44596700
Si	1.47287700	-0.00098500	-1.76738900	Si	-0.14243600	0.27078000	2.21735400
Si	-1.91916600	-0.00431600	-1.75456300	Si	2.13645200	-1.53755300	-0.59461900
Si	-1.74341800	-1.93825100	0.00995400	B	0.42639300	-0.32339900	-1.05439200
Si	-3.20247600	0.00265800	0.33734600	Si	-0.09163000	-2.57085100	-0.46414400
Si	-1.73911800	1.94075400	0.00393400	Si	0.36034800	2.52617700	-1.15201400
Si	0.23641300	1.18848900	1.82474400	Si	-1.10420800	2.06921900	0.72354300
Si	0.23189800	-1.19103400	1.81668000	Si	-2.74158200	0.48238600	-0.17899400
B	1.73123900	0.00129400	0.89970400	Si	2.28284300	0.98689700	-0.95056600
10C				10D			
	X	Y	Z		X	Y	Z
B	-0.49459000	-0.66013500	0.77878800	B	-0.51698500	0.54866900	-0.86733300
B	1.00695400	-0.46720400	-1.41134200	B	1.92716100	-1.06623700	0.01348300
B	-0.81062800	0.91137500	0.02936900	B	-0.79836000	-0.94654400	0.02422100
Si	-2.46795300	0.47139400	-1.26557000	Si	1.47410600	0.84142300	1.55024600
Si	-2.37868800	0.28642500	1.36113500	Si	-2.12281400	1.78890800	-0.03667900
Si	1.49901800	-1.05930000	1.52615200	Si	0.60380100	-2.55518400	0.05470900
Si	0.01116000	0.98539800	1.95219400	Si	0.25855000	2.35560000	-0.05800000
Si	0.29581900	-2.29770100	-0.35238100	B	-0.50436700	0.59001000	0.83625100
B	-0.61762300	-0.53386200	-0.94748900	Si	-0.06825000	-1.10626000	1.98260300
Si	-2.17653800	-1.76657800	-0.05336200	Si	-0.09905700	-1.20764200	-1.93640900
Si	-0.12213800	1.22105400	-1.96794100	Si	-2.41029100	-0.44848400	-1.27693000
Si	0.53192700	2.54150000	0.06567000	Si	-2.39728900	-0.37587400	1.31735500
Si	2.79149400	-1.07232700	-0.82346400	Si	1.45591900	0.74320000	-1.57672800
Si	2.34300100	0.95793100	0.11137800	Si	3.26695100	0.27649300	-0.02253200



11A				11B			
	X	Y	Z		X	Y	Z
B	-0.03232300	0.30451900	1.26954700	B	0.72454100	-0.12672600	-0.80411600
B	-1.07471000	0.74569300	-1.21400600	B	-1.82002700	-0.86243400	0.41874100
B	0.72794300	-0.93590900	0.24217800	B	0.95998700	0.87353500	0.61276800
Si	2.45119800	0.22301700	-1.15786200	Si	2.81619900	0.06994400	1.20997500
Si	1.99006200	0.53134700	1.41141800	Si	2.54235000	1.00405400	-1.09058600
Si	-2.24047800	0.41274100	1.48316600	Si	-1.16042700	-0.16296000	-1.80913400
Si	-0.91572600	-1.55727600	1.56820800	Si	0.19716500	1.87206300	-1.21910800
Si	-0.71719600	2.22803700	0.30983600	Si	0.05432200	-2.10410600	-0.79287200
B	0.47115000	0.75753000	-0.38187300	B	0.92357500	-0.84650100	0.80267300
Si	1.99339000	2.31506300	-0.20224800	Si	2.43593100	-1.44408800	-0.73779800
Si	0.20396100	-0.61676400	-1.93270100	Si	-0.74776900	0.15451100	1.93789500
Si	-0.35263500	-2.58515600	-0.60327300	Si	-0.30079400	2.47087100	1.16090000
Si	-2.92166900	1.27662600	-0.81971400	Si	-3.40763600	-0.49943300	-0.72731700
Si	-2.28217900	-1.03777000	-0.56027900	Si	-2.08243400	1.17341700	0.17880800
Si	2.75839500	-1.50123400	0.53350500	Si	-0.62836200	-2.19065800	1.52135500
11C				11D			
	X	Y	Z		X	Y	Z
B	0.71104200	-0.51933200	0.62899100	B	-0.23155700	-0.63035100	0.58663300
B	-0.21202300	0.97099100	0.27645200	B	0.62080100	1.00141100	0.70232800
B	-1.47234600	0.38797300	-0.96935200	B	-0.27720500	0.61505300	-0.84053800
Si	-1.14401500	-1.54564100	-1.74287800	Si	2.10318800	-0.60379700	-1.72815400
Si	-0.66902000	-2.20625500	0.85984200	Si	-0.91414400	-2.52458200	-0.21502600
Si	1.56462200	1.23706300	1.55702100	Si	-0.43051700	2.61263300	-0.09118900
Si	-0.48104500	0.04792400	2.22278900	Si	1.47931600	-1.95049800	0.27824600
Si	2.30437200	0.17193700	-1.46042400	B	0.14847300	-0.99813400	-1.14860300
B	0.22725500	-0.03762900	-1.06510700	Si	1.59628000	1.76719700	-1.08710100
Si	1.27004800	-1.98925400	-0.66637200	Si	-1.06430000	0.81835500	1.94573100
Si	-1.43838800	2.41087000	-1.00188900	Si	-2.47490800	-0.88259100	0.72919800
Si	-2.26959100	1.09466500	0.89840400	Si	-1.86381600	-0.60989300	-1.74498200
Si	-2.76301700	-1.05919700	-0.10068700	Si	1.19278800	-0.36473900	2.18254900
Si	1.02633700	2.19322500	-0.89672100	Si	-2.49150200	1.30228600	-0.50629600
Si	2.86615100	-0.64176500	0.73413400	Si	2.77457500	0.43992100	0.48708800



12A				12B			
	X	Y	Z		X	Y	Z
Si	2.24366300	1.02888100	0.86409800	B	0.81357400	-0.71552200	0.73257900
Si	3.03546000	-0.35622100	-0.93253700	B	-1.55143300	0.49398800	-0.53498000
Si	1.24429300	1.15362800	-1.70455000	B	0.05105800	0.85118100	0.30930100
Si	1.91043300	-2.35192300	0.08540400	Si	1.74977400	-0.05571100	-1.67601600
Si	0.74604400	2.69442600	0.17223100	Si	-0.68138700	-2.20392200	0.82505100
Si	-0.36271000	-2.20537500	-0.86528600	Si	-2.69769600	-0.65930700	0.96145900
Si	-1.94212500	1.50507100	-1.45612200	Si	1.60989000	2.07971500	-0.55256300
Si	1.05941900	-0.78742600	1.79586800	Si	1.89481600	0.98184300	1.60306500
Si	-1.54863400	2.06220600	1.10200800	Si	-2.11751100	-1.38793900	-1.24823900
Si	-1.31899300	-0.16404100	2.18548800	Si	-0.21245300	0.02465300	2.41066800
Si	-2.24593800	-1.84683800	0.65752600	Si	-0.95567400	0.27800200	-2.50495300
Si	-2.41280200	-0.79885900	-1.57157200	Si	-0.86350800	2.45596700	-0.83724700
B	-0.42112700	-0.02536000	-1.15613900	Si	-1.82300600	1.58786400	1.24964100
B	-1.70745300	0.18642900	0.12909800	Si	1.40325500	-2.30328100	-0.53982500
B	0.00635100	0.63090400	0.51138400	Si	2.97874400	-0.79603500	0.39723800
B	0.97952300	-0.60585400	-0.41550000	B	-0.11187900	-0.63482100	-0.75407300
12C				12D			
	X	Y	Z		X	Y	Z
B	-0.06232700	-0.91519300	0.97456300	Si	1.86703800	1.51368400	-1.28774300
B	0.82363300	-0.25706400	-0.43610000	Si	-1.91380600	0.45382800	-1.22489100
B	-0.59614600	0.82053000	-0.92366600	Si	-0.52313600	2.45378700	-1.37496700
Si	1.43726400	-0.10026100	2.34279800	Si	0.89291700	-2.27580800	-0.57129700
Si	-1.43159000	-0.96587200	-1.87374900	Si	-2.25183000	-1.57312900	0.52929300
Si	-0.89275800	0.41840800	2.40989800	Si	1.79572800	1.48035500	1.10771700
Si	1.62281700	-2.04736000	0.52918700	Si	2.94833400	-0.84688600	-1.02633300
Si	2.38413900	1.20095800	0.36409200	Si	-0.56245800	2.20864400	1.35639900
Si	0.55908200	0.20186600	-2.52335600	Si	2.50920600	-0.72866100	1.46998100
Si	-2.77111200	0.60660200	-0.75351900	Si	-3.20183700	0.57686100	0.78901200
Si	-0.70889500	-2.66475300	-0.08201400	Si	-0.12044500	-1.55804300	1.73253900
Si	0.60264100	2.62217200	-0.69723600	Si	-1.37186300	-1.78836400	-1.74496500
Si	-2.20165600	-1.12465200	0.89926600	B	-1.13975600	0.20611800	1.15687700
Si	2.62134800	-0.59246000	-1.27167200	B	0.01721900	0.94158300	-0.13562500
Si	-1.38776900	2.23475600	0.54038000	B	-0.37025400	-0.72634100	-0.20505400
B	0.30101100	0.94140000	0.70979300	B	1.30281200	-0.18691000	-0.12948500



13A				13B			
	X	Y	Z		X	Y	Z
B	-1.38207000	0.78882800	0.00730500	B	0.81768800	-0.00273200	-1.19722600
B	-0.22313200	-0.19936300	-0.87820200	B	-1.54097500	0.00140300	0.55315800
B	1.41794000	0.08696800	-0.00494200	B	-0.02326100	-0.90334800	0.16474100
Si	-2.61339000	-0.47063100	1.24743600	Si	1.99613900	0.00042000	1.16868300
Si	1.26446800	0.87324700	-1.99089900	Si	-0.48835900	1.41938500	-2.04891600
Si	-1.18872400	1.46191500	1.95549600	Si	-2.68742500	-0.00749300	-1.34055100
Si	-2.60812200	-0.47428700	-1.23611800	Si	1.09041800	-2.09143000	1.57374000
Si	-0.91999700	-2.26325900	1.19287900	Si	1.56702800	-2.01851400	-0.92449400
Si	1.33296600	-1.49558000	-1.65263000	Si	-1.99950600	1.93594900	-0.09232300
Si	1.91061300	2.20526600	0.00242700	Si	-0.49217000	-1.41675400	-2.04991600
Si	-1.20287200	1.46833000	-1.94264100	Si	-1.18229000	1.33988500	2.14557500
Si	1.31926800	-1.52521400	1.64218600	Si	-1.18459800	-1.32192700	2.15546500
Si	-0.52288300	2.72345200	0.00640200	Si	-1.99377000	-1.93856900	-0.08010800
Si	-0.91054000	-2.26364200	-1.22080500	Si	1.57832800	2.00843300	-0.93049800
Si	1.28322800	0.84405200	1.99206700	Si	2.97702400	-0.00711800	-1.02569600
B	-0.21518600	-0.19820200	0.87857700	B	-0.02630600	0.90735700	0.15849800
13C				13D			
	X	Y	Z		X	Y	Z
B	-0.28031400	0.09617200	1.06982200	B	1.53975500	0.37751200	-0.19378100
B	-0.14661300	0.68132800	-0.64668900	B	-1.62927900	0.31789400	0.23951400
B	0.48847700	-0.57917500	-1.74659000	B	0.42970900	-0.84497300	-0.58580600
Si	-1.90675200	1.58046400	1.51510900	Si	0.89900700	-0.90249500	1.42976200
Si	1.96379200	-1.45356500	-0.37602600	Si	1.00239800	2.29263800	-1.05590000
Si	-2.05990000	-0.84751600	1.82973800	Si	-1.50910900	1.91368900	-1.09233800
Si	0.65663900	1.88816200	1.30916400	Si	0.86851100	-2.84533000	0.00105600
Si	-1.95042800	1.94836800	-1.01874500	Si	2.50617800	-1.34703100	-1.16255300
Si	1.78475600	0.87065900	-1.55690400	Si	-0.87167200	2.00978300	1.31618200
Si	0.20650500	-2.59740600	-1.31424700	Si	1.04253800	0.24055800	-2.32802200
Si	1.71212100	-0.22346200	1.94291800	Si	-1.23175500	-0.07784800	2.30241700
Si	-1.60392800	-0.28148100	-2.08086500	Si	-3.01098400	-1.05960000	0.97385300
Si	0.14218500	-2.02564700	1.32635000	Si	-2.95243300	-0.01684400	-1.43751500
Si	0.35843700	2.75104500	-0.89837900	Si	1.68690100	1.96039700	1.16919700
Si	-2.07832500	-1.99371700	-0.38984400	Si	3.11815100	-0.14053900	1.08437000
B	-1.65161300	0.08204900	-0.01154900	B	-0.87433100	-0.15667900	-1.44650100



14A				14B			
	X	Y	Z		X	Y	Z
B	-1.44326100	0.90278900	-0.15938300	B	-1.46443900	0.42504600	-0.00050600
B	0.25338300	-1.43434800	0.14121400	B	-0.00010400	-0.26521400	-0.87349900
B	-0.04454300	0.01144500	-0.88467800	B	1.46323100	0.42457200	0.00051500
Si	1.07596600	1.81076400	-0.61376200	Si	-1.90004400	-1.11197200	1.65487000
Si	-2.11689700	0.29070900	1.72465100	Si	1.22636500	1.20280700	-1.95946300
Si	-1.47914200	-2.70268000	-0.09197800	Si	-1.22537000	1.20006900	1.96087000
Si	1.77943400	0.13408600	-2.08669800	Si	-1.89931400	-1.10613500	-1.65698800
Si	-1.67643900	0.57891700	-2.16308300	Si	-0.00097300	-2.45727100	1.20054200
Si	-0.75896700	-1.78287600	2.00545600	Si	1.89909900	-1.10846500	-1.65484200
Si	-2.84808200	-0.64735400	-0.44153000	Si	1.24528700	2.65891800	0.00227200
Si	1.62551200	-1.06149400	1.76898800	Si	-1.22334300	1.20528400	-1.95939700
Si	2.29930500	-1.76254800	-0.46173500	Si	1.89862300	-1.11150300	1.65435100
Si	0.02278000	-1.82782300	-1.88027300	Si	-1.24465000	2.66038700	0.00205500
Si	-0.87054500	2.33894200	1.38254800	Si	-0.00067800	-2.45598900	-1.20615200
Si	-1.10753400	2.81982200	-1.00939700	Si	1.22596400	1.19994900	1.96130500
B	-0.09432100	0.14070500	0.90078900	B	-0.00130700	-0.26490600	0.87429000
Si	1.44725800	1.35630500	1.83095800	Si	3.40766200	-0.44554600	0.00060500
14C				14D			
	X	Y	Z		X	Y	Z
B	-1.44518000	0.40524500	0.00394100	B	-1.42734100	0.86348000	-0.28420700
B	0.00929800	-0.26530500	-0.87697100	B	-0.19014600	-0.27904000	-0.83143000
B	1.48571800	0.33201600	-0.00234800	B	1.22546500	-0.03893600	0.32881200
Si	-1.88748200	-1.06671200	1.73186300	Si	-2.97681300	-0.22186400	0.75672800
Si	1.15839300	1.29987400	-1.95576600	Si	1.44329600	0.46795300	-1.82220000
Si	-1.21727300	1.25887000	1.95352600	Si	-1.60365500	1.59921700	1.62653800
Si	-1.88530400	-1.07273600	-1.72819100	Si	-2.48565400	-0.27943300	-1.78491000
Si	-0.01124100	-2.43329600	1.22723400	Si	-1.46769000	-2.13487900	1.36225000
Si	1.79156300	-1.05402900	-1.91608100	Si	1.05204600	-1.93299200	-1.63451000
Si	1.47965400	2.63125700	0.00128200	Si	1.68288500	2.05587500	0.45136900
Si	-1.22680300	1.25547600	-1.94938400	Si	-0.75260900	1.47309900	-2.14369300
Si	1.79071100	-1.06319900	1.91318000	Si	0.76683200	-1.44310700	2.03470400
Si	-0.99187900	2.67826600	0.00052100	Si	-0.59041800	2.90680700	-0.20195900
Si	-0.00574800	-2.43362900	-1.23067500	Si	-1.15408900	-2.19154100	-0.99969300
Si	1.16733600	1.29082300	1.95490700	Si	0.67633000	0.92509300	2.26970600
B	0.01117000	-0.26759000	0.87340000	B	-0.61621200	-0.23449500	0.85714900
Si	3.16452800	-0.92029300	-0.00156200	Si	2.43926300	-1.77864300	0.36616100



15A				15B			
	X	Y	Z		X	Y	Z
B	1.47010900	-0.61571800	-0.08188100	B	1.41758400	0.32991000	0.29455900
B	-0.03385300	0.09840300	-0.87147700	B	-0.19382600	-0.17879000	0.94006000
B	-1.32993200	-0.03640000	0.50600800	B	-1.26750300	0.33568300	-0.57381000
Si	2.41815800	1.10489200	1.14251100	Si	3.27610200	-0.65302700	0.36500300
Si	-1.48739300	-1.01254500	-2.27829300	Si	-1.63438500	1.00645500	1.83936100
Si	1.55188600	-0.91054000	2.05793500	Si	1.81587100	-0.71643300	-1.78320700
Si	1.88160400	0.27348800	-2.11169400	Si	1.77533300	-0.80245200	2.22365400
Si	0.68749900	2.69097500	0.76348200	Si	0.41291000	-2.72011900	-1.19252000
Si	-1.60058100	1.28047400	-1.74555300	Si	-1.88613300	-1.36286100	1.91811600
Si	-1.32847400	-2.11905900	1.06683500	Si	-0.85492100	2.30689700	-1.30338200
Si	0.68512800	-1.78377600	-1.75312800	Si	0.66868200	1.42120100	2.21790100
Si	-1.28322100	1.71989600	1.82712100	Si	-1.54877200	-1.42281900	-1.85586100
Si	0.96751500	-2.74856400	0.44315500	Si	1.11386100	2.56638000	0.16070100
Si	0.50366800	2.15980800	-1.57845200	Si	0.14778900	-2.26758100	1.14519300
Si	-0.71278900	-0.44710400	2.63279600	Si	-0.23143300	0.44212400	-2.57494800
B	0.32498600	0.51488900	0.82814800	B	0.14332800	-0.69591500	-0.60376500
Si	-2.99878700	1.21957400	0.19408100	Si	-3.08247100	-0.76524200	-0.18648900
Si	-2.93798100	-1.18658500	-0.32038100	Si	-2.84200700	1.67591800	-0.12757600
15C				15D			
	X	Y	Z		X	Y	Z
B	-0.68121200	0.96701400	0.71127200	B	-1.37600300	0.51194100	-0.17048900
B	0.84344700	0.54488700	-0.23431100	B	0.77535300	-1.39189600	0.29808200
B	1.03682100	-1.21365600	0.04537900	B	0.10322000	-0.21399500	-0.81496700
Si	-3.71589300	-0.67790400	-0.18843700	Si	0.72195300	1.75831100	-0.92122500
Si	2.92473800	-0.49869100	0.37564400	Si	-1.59216000	0.13578500	1.96658000
Si	-1.83852900	-0.62245700	1.35094100	Si	-1.00187100	-2.76521900	0.27197100
Si	-0.91802500	2.88860100	-0.21324600	Si	1.65227300	0.17609900	-2.34039100
Si	-1.83373600	-0.86945500	-1.85167600	Si	-3.09479200	0.87123800	-1.46524600
Si	2.15569700	-1.53544300	-1.77932400	Si	-0.08589200	-1.73132600	2.24957700
Si	1.46706900	-1.13874200	2.22748300	Si	-1.61206600	-0.99317600	-1.68838700
Si	0.93587400	1.84838800	1.55915900	Si	2.10483000	-0.70432800	1.81176900
Si	-0.02267800	-2.50226500	-1.24167900	Si	2.85301100	-1.20655200	-0.43438300
Si	-0.29012100	0.41487300	2.98514000	Si	0.63516700	-2.19407600	-1.60484700
Si	-0.59090100	1.14874100	-1.87515600	Si	-0.74877800	2.34790100	1.63743400
Si	-0.22383400	-2.45724400	1.21056700	Si	-1.47288300	2.63009400	-0.66056700
B	-0.50515900	-0.55296200	-0.24168100	B	0.21004700	0.16195500	0.87041400
Si	1.68948900	0.85575900	-2.20128300	Si	1.62878000	1.63719300	1.39644500
Si	-2.61863400	1.38040700	-0.24981900	Si	3.12639100	1.28146900	-0.61274400

Table S2. Cartesian coordinates for stable isomers of B₄Si₄₋₁₅ clusters.

B ₄ Si ₄							
4A				4B			
	X	Y	Z		X	Y	Z
Si	-1.97096900	-0.40594200	-0.24971100	B	-0.10090800	-0.20032100	-0.66072500
Si	0.00041100	-1.68080700	0.05675600	B	-1.08317500	-0.25252200	1.13689300
Si	-0.00007800	0.68370400	1.29509800	B	0.47130200	0.22799400	1.01722000
Si	1.97106800	-0.40530800	-0.24978400	Si	1.78518900	-1.17612500	0.08957600
B	-0.00024200	0.25045900	-0.84088700	Si	1.44494000	1.16769600	-0.54274400
B	-0.00035600	2.09485900	-0.63628500	Si	-1.04603500	1.54117900	0.28873600
B	1.33531800	1.35916000	-0.45472500	B	-0.03908200	-1.34452600	0.69299800
B	-1.33593000	1.35891000	-0.45470900	Si	-1.91557100	-0.97225900	-0.61642000
4C				4D			
	X	Y	Z		X	Y	Z
Si	-1.40179900	1.31227300	-0.54213400	B	0.38553800	-0.29357800	-0.91132600
Si	2.56075600	0.52450700	0.26503400	B	0.39316300	-0.25881700	0.92072800
Si	-2.39879900	-0.66692900	0.42037800	B	-0.51480100	-1.46704000	0.03228700
Si	1.18542500	-1.20575000	-0.62865200	Si	2.30829000	-0.13333100	-0.00152000
B	-0.57176000	-0.10989400	1.06264800	Si	-1.54062800	-0.10371700	-1.23436700
B	0.42241200	0.67364000	-0.33949600	Si	-1.53098200	-0.04657800	1.23986000
B	-0.65145200	-0.62737000	-0.63989900	Si	0.30111200	1.57929600	-0.02959600
B	0.95316600	0.16414200	1.27579400	B	1.03028300	-1.60844300	0.03005400
B ₄ Si ₅							
5A				5B			
	X	Y	Z		X	Y	Z
B	-0.82936900	-0.02347400	1.02888400	B	0.01245900	-1.45680100	-0.60912800
B	0.82981100	-0.02202500	1.02756200	B	-0.76097000	-0.00130900	-0.97015700
B	-0.00152400	1.38584400	0.75453200	B	0.88078500	-0.00113200	-0.90134700
Si	0.00145300	-1.84810000	0.47739800	Si	-1.92188500	1.32936600	-0.00507600
Si	-1.75314300	1.50485900	-0.11038200	Si	1.87955700	-1.53317200	-0.00958300
Si	1.74944200	1.50833000	-0.11152800	Si	1.87717200	1.53367300	-0.00892400
Si	-1.95283600	-0.84415400	-0.52546300	Si	0.03700500	0.00150400	1.13347800
B	-0.00049200	0.11764700	-0.58792300	B	0.01225900	1.45460400	-0.61493900
Si	1.95564700	-0.84164600	-0.52397200	Si	-1.92346800	-1.32971500	-0.00433300
5C				5D			
	X	Y	Z		X	Y	Z
B	-0.69308800	0.11786400	-0.95491600	B	0.47807500	0.07262000	-0.81657700
B	0.96266300	0.08589800	-0.94100900	B	1.07143200	0.58581700	0.87181600
B	0.04438200	-1.40658600	-0.89621800	B	-0.47979800	0.07629400	0.81987200
Si	-1.99398000	0.99315600	0.25141100	Si	-2.56912800	0.21152000	0.31327600
Si	0.17686000	-0.35890400	1.08282500	Si	-1.04886400	-1.47467600	-0.58936700
Si	-1.77782600	-1.48968500	-0.07494100	Si	2.56574100	0.20363100	-0.31423900
Si	0.23192700	1.87828800	-0.31839500	Si	1.03972800	-1.48672100	0.58589300
B	1.57639400	-1.45197400	-0.50498800	Si	0.01234100	2.06964200	0.00060100
Si	2.68789400	-0.07471300	0.23664600	B	-1.06920300	0.59976400	-0.86437100

B₄Si₆

6A				6B			
	X	Y	Z		X	Y	Z
B	0.67057000	0.44993900	-0.79919400	B	-0.83004100	0.29009100	-0.92051400
B	-0.69819600	-0.45191500	-0.82220900	B	0.83316500	0.23084200	-0.68515100
B	-0.67148000	0.44779800	0.79662500	B	-0.10843600	1.56688200	-0.03003600
Si	1.00930000	-1.73380400	-0.83994500	Si	-2.37851200	-0.88638600	-0.25091100
Si	1.03030100	1.74093500	0.82398100	Si	-0.66544700	-0.15357500	1.26775600
Si	-2.53160200	-0.00935200	0.00314900	Si	-2.07973700	1.63981400	-0.03455500
Si	2.53160000	-0.00703600	-0.00698700	Si	-0.09433100	-1.64798700	-0.79262500
B	0.69888400	-0.44975100	0.82034900	B	1.50527200	1.62212100	0.01104400
Si	-1.00838100	-1.73228500	0.84253500	Si	2.97711700	0.59242600	-0.53055200
Si	-1.03114100	1.74294500	-0.82115000	Si	1.74092600	-0.86926900	0.92112100
6C				6D			
	X	Y	Z		X	Y	Z
Si	-1.22388400	2.06084500	-0.44782800	B	-0.42453100	-0.11721200	-0.66806000
Si	1.03425500	1.46476200	-0.41758500	B	0.83954800	0.34433600	0.57636700
Si	1.03654500	-1.45959900	-0.42015400	B	0.15392300	-1.30638300	0.53067700
Si	2.81498400	0.00040700	0.28616000	Si	-2.32014900	0.62641600	-0.62682600
B	-0.46041000	0.83657400	1.04910900	Si	-1.08322500	0.19560000	1.49982300
B	-0.45855100	-0.83646600	1.04979500	Si	-1.72540600	-1.69411000	-0.13276700
B	0.98593100	0.00182300	1.10540600	Si	-0.22823100	1.93470500	-0.17262000
B	-0.50593900	0.00003600	-0.60396100	B	1.73110100	-1.13955200	0.72329700
Si	-1.21713000	-2.06424000	-0.44672000	Si	3.04303400	0.15631400	0.39865200
Si	-2.28799500	-0.00287700	0.51743100	Si	1.49253200	-0.42649200	-1.38136300

B₄Si₇

7A				7B			
	X	Y	Z		X	Y	Z
B	-0.74952100	0.59282400	0.61594800	B	-0.63945300	0.39301600	0.65912400
B	0.70086700	0.36890300	-0.35376300	B	-0.66449200	-0.88640500	-0.62833700
B	0.15953000	-0.88464200	0.92092900	B	0.66141800	-0.88895600	0.62356500
Si	-2.64595900	0.70920300	-0.03639200	Si	2.55396000	-0.34933700	-0.17018900
Si	-0.99582000	-0.92910600	-1.07901600	Si	1.30084200	0.99772200	1.46160100
Si	-1.80250100	-1.18664100	1.25653000	Si	-2.55509000	-0.34667600	0.16942700
Si	-0.74695200	1.51511200	-1.32325100	Si	-1.07151700	-1.65626800	1.36627600
B	1.75489400	-0.75545100	0.88290800	Si	-1.30173800	1.00419700	-1.45771900
Si	2.73739800	0.63710000	-0.25955100	B	0.64065000	0.39487700	-0.65753000
Si	1.59305500	-1.52626500	-0.94543100	Si	0.00504200	2.36025600	-0.00011900
Si	1.19443300	1.02287100	1.64924500	Si	1.06917100	-1.65722600	-1.36814100
7C				7D			
	X	Y	Z		X	Y	Z
B	0.66261800	-0.57414600	0.79954100	B	-0.02585300	1.41587900	-0.21472800
B	0.10163900	0.98020800	0.88464300	B	0.49313300	-0.19095900	-0.70585700
B	-0.51366800	0.11958100	-0.64055500	B	-0.69007300	-0.01763100	0.70257900
Si	2.14018600	0.94950200	0.78592300	Si	0.51965800	-1.70956300	0.94806800
Si	-0.20868300	-1.94214600	-0.48412400	Si	2.50455600	-0.70837600	-0.27051200
Si	-1.66994100	1.65038200	0.17318900	Si	1.25986100	0.71005800	1.42295800
Si	2.28941000	-1.45405000	-0.20322300	Si	1.83537100	1.42417200	-0.99624500
B	1.16218200	0.00145800	-0.96842600	Si	-1.93447100	1.84237000	0.16891800
Si	0.63236000	1.94080500	-1.06552000	Si	-2.66638900	-0.44163000	0.26283700
Si	-1.34900800	-0.58112700	1.51738800	B	-1.14273200	0.32873900	-1.01282900
Si	-2.33888500	-0.75161500	-0.75049100	Si	-1.03089800	-1.66561300	-1.09644000

B₄Si₈

8A				8B			
	X	Y	Z		X	Y	Z
B	-0.89290000	-0.02039300	-1.26808800	B	-0.03161000	-1.07519200	0.24244000
B	-0.07972400	1.38107900	-0.80276500	B	-0.99832200	0.59888100	0.82041700
B	0.75824800	0.08298900	0.18090900	B	-0.73198300	0.29853900	-1.22756400
Si	-2.05325500	1.41732200	-0.02278500	Si	0.96577100	0.31387100	1.56720900
Si	-0.31966600	-1.88726700	-0.14993300	Si	-0.02982900	-1.54792900	-1.83780500
Si	1.78978600	1.84648300	-0.54468200	Si	-2.17158900	1.56340000	-0.65521300
Si	-2.51853000	-0.95489900	-0.63350000	Si	1.89648700	-1.50810600	-0.30289400
B	-1.03997800	-0.20109300	0.77700900	B	0.89286700	0.12387000	-0.97785500
Si	0.00156100	1.53152000	1.53885600	Si	0.15131000	2.00783500	-0.28279300
Si	1.05452100	-0.06663100	-1.93692000	Si	-2.06223400	-1.03385300	-0.10111700
Si	2.04116200	-1.47609300	0.10454200	Si	-0.89462000	-0.94334700	2.16655000
Si	0.45240400	-0.85421500	2.04190000	Si	2.45507800	1.16738000	-0.14587900
8C				8D			
	X	Y	Z		X	Y	Z
B	-0.45412300	0.02187600	0.06333800	B	0.27608500	-1.13811900	-0.36852000
B	0.17717800	1.61895800	-0.13118100	B	-0.77338300	0.24514600	-0.78762900
B	0.90485600	0.23726000	-1.09732900	B	0.37001500	0.54527100	0.63044100
Si	2.37929000	-0.80858600	0.05489600	Si	-1.37577700	1.59935600	0.90233100
Si	0.18150700	-1.78172400	-1.04223500	Si	-2.82239600	0.11010800	-0.47984500
Si	-1.84631300	1.69348500	-0.03848700	Si	-1.06893000	-0.87007200	1.41314100
Si	-0.97780100	0.21590000	-1.98721800	Si	-1.51848800	-1.80672300	-0.96104300
Si	-0.65700200	0.77608800	2.04757900	Si	2.33514400	-1.17336000	-1.00515600
B	1.03842600	0.50149900	0.95174800	Si	2.34241700	1.08065800	0.25883300
Si	0.17651700	-1.46175300	1.52988800	B	0.92889900	0.26883100	-1.15134500
Si	2.19140700	1.66432400	-0.43868100	Si	0.31457900	2.15934900	-0.91166300
Si	-2.04272600	-1.14758900	-0.04951900	Si	1.50716000	-1.07114900	1.38235000

B₄Si₉

9A				9B			
	X	Y	Z		X	Y	Z
B	0.65144900	0.21651100	0.87479300	B	-0.45705600	-0.93444900	0.30072100
B	-1.55663200	0.55113200	-0.00034000	B	1.08177700	0.28954500	-1.42494100
B	-0.37637600	-0.96314900	0.00003000	B	-0.49801600	0.79008000	0.55871400
Si	-0.58200200	1.92462700	-1.37398200	Si	-2.22405400	1.35974500	-0.62018000
Si	2.58924100	-0.25883300	0.00298800	Si	-2.18664900	-0.25681900	1.42195100
Si	-2.54153000	-1.13212300	0.00083300	Si	1.56640600	-1.51020200	0.65446000
Si	1.46692800	1.99266300	0.00076500	Si	0.17405100	-0.32599400	2.26615500
B	0.65147000	0.21699700	-0.87423800	Si	0.35099200	-1.71397600	-1.49844700
Si	-1.07902700	-0.41327000	-1.95667200	B	-0.54629600	0.15513900	-1.07348400
Si	-1.07929000	-0.41067300	1.95696000	Si	-2.15369500	-1.21917800	-1.00311600
Si	1.01576500	-1.81991200	1.32411400	Si	0.20784400	2.14334500	-0.90100500
Si	1.01860700	-1.81647600	-1.32603600	Si	1.51613300	1.28919300	1.02479200
Si	-0.58366000	1.92632200	1.37094200	Si	2.89882600	0.12663100	-0.75925600
9C				9D			
	X	Y	Z		X	Y	Z
B	-0.64821300	0.68424700	0.59620300	B	0.31662900	-1.01713500	-1.10593700
B	-0.81868400	0.05962300	-1.11410800	B	-0.97470500	-0.45510400	0.11944100
B	0.02874900	-1.01019100	0.20018000	B	-0.24766700	0.53948600	-1.12413800
Si	2.05947600	-1.51144700	0.46457700	Si	0.66590500	2.36626600	-0.72803200
Si	0.65969800	-0.13488500	2.02847000	Si	1.86747700	0.37142600	-1.42695700
Si	-2.66375300	0.47928300	-0.16377100	Si	-0.38325000	-2.46191000	0.15779700
Si	-1.52788400	-1.03550800	1.55857400	Si	-1.54539100	-1.09922200	-1.86198800
Si	-1.02295400	2.22008800	-0.88343200	Si	-1.92456300	0.62707500	1.81739400
B	0.57202500	0.88994600	-0.89369300	B	-0.31126300	1.06877300	0.66553600
Si	0.81618700	2.11495700	0.78064400	Si	0.15708700	-0.56983700	1.93182300
Si	0.89024700	-1.06640300	-1.73705200	Si	1.95574700	-1.46150700	0.17318600
Si	2.61735100	0.58920700	-0.67821200	Si	1.81376700	1.02852200	1.08206900
Si	-1.51903900	-1.87801600	-0.93714900	Si	-2.17213200	1.15060800	-0.62918500

B₄Si₁₀

10A				10B			
	X	Y	Z		X	Y	Z
B	-0.04995100	0.90295200	0.64558000	B	-0.51111300	-1.04282000	0.28924200
B	-0.04945700	-0.90325700	0.64345900	B	-0.50954200	0.27477300	-1.05291800
B	1.50039300	-0.00008400	-0.70490200	B	0.90110500	0.00342400	0.00046200
Si	-1.73843900	-1.96824300	0.03201300	Si	-2.23161300	1.45541400	-0.40373300
Si	-3.28105400	0.00143300	-0.13673700	Si	-0.02674300	-0.60431300	2.32933700
Si	-1.73626000	1.96911300	0.03113900	Si	1.38073700	0.52162400	-2.01315800
Si	-1.71408400	-0.00045800	1.71504300	Si	-2.22552100	-0.38373400	1.46930800
Si	1.59864300	-0.00052500	1.70885000	B	-0.50932000	0.77562100	0.76274200
Si	1.69471600	-1.94779800	0.04521200	Si	-0.03751800	2.32405800	-0.64271400
Si	3.35302800	0.00117200	0.00636700	Si	-0.02022900	-1.71444800	-1.68387000
Si	1.69308000	1.94809300	0.04534100	Si	1.37443900	-2.00451300	0.55562900
Si	0.03872400	1.23472400	-1.73758900	Si	1.37715800	1.49159100	1.45325300
Si	0.03788100	-1.23737800	-1.73601800	Si	-2.22243400	-1.08744400	-1.06843100
B	-1.25044400	0.00001600	-0.51027600	Si	2.85632000	-0.00216400	0.00454800
10C				10D			
	X	Y	Z		X	Y	Z
B	-0.54898100	0.70972500	0.73165000	B	0.65766400	-0.84596500	0.30116300
B	-0.55530000	0.50894700	-0.98674000	B	0.52426100	0.19600100	-1.10997800
B	-0.79655700	-0.89984500	0.06555400	B	0.33596700	0.87144600	0.56219400
Si	0.44564900	-2.59333500	0.29376200	Si	-1.78804500	1.26430000	0.97995200
Si	-0.07463200	-0.84182000	2.04675700	Si	-0.25959600	-0.36704200	2.15638900
Si	-2.17682000	1.76077100	-0.28335200	Si	2.54700800	-0.67248800	-0.78308000
Si	-2.44582000	-0.24251800	1.25337700	Si	2.09742800	0.25902000	1.57520500
Si	0.23038900	2.39367500	-0.37434800	Si	0.77755000	-2.28394000	-1.25670800
B	1.11230200	0.57404700	-1.17221800	B	-0.70312400	-0.94965200	-1.04192000
Si	1.40998600	1.12687400	1.48550200	Si	-0.80210300	-2.34869800	0.56966400
Si	0.10040400	-1.28461000	-1.84490200	Si	-1.62802700	0.79135100	-1.56489300
Si	2.17853300	-1.06147900	-0.17402000	Si	-2.68423600	-0.78851100	-0.20196900
Si	-2.35284100	-0.58898300	-1.34301400	Si	1.88639600	1.78361500	-0.55460700
Si	2.96677100	1.01254200	-0.57342000	Si	-0.43736300	2.62245500	-0.45975900

B₄Si₁₁

11A			11B				
	X	Y	Z		X	Y	Z
B	-0.85844100	-0.46493200	-0.07927200	B	0.71676700	-0.11941900	-0.87214700
B	0.85851500	-0.46486500	-0.07937900	B	-1.75792800	-0.85986400	0.40511100
B	-0.00007900	1.02035500	0.07179900	B	1.04852000	0.85388100	0.55674500
Si	1.73367700	1.19028200	1.36015400	Si	2.93759000	-0.00314100	1.04740900
Si	0.00011000	-2.16475500	1.03671500	Si	2.45223400	1.10945700	-1.10521400
Si	2.22694800	-1.21904600	1.25647300	Si	-1.21591100	-0.11901700	-1.80221600
Si	-1.73365600	1.18951200	1.36042700	Si	0.10776500	1.91051800	-1.17680000
Si	-2.30547000	-1.06233200	-1.36565900	Si	-0.08775400	-2.08349400	-0.80325100
Si	1.87256700	1.33250400	-0.97034000	B	0.99223700	-0.87196600	0.73084300
Si	2.30608200	-1.06205300	-1.36521900	Si	2.32280100	-1.53343300	-0.80506500
Si	-0.00047200	2.92870800	-0.70824000	Si	-0.53737500	0.10593200	1.83789900
Si	0.00041400	-2.05726100	-1.33328000	Si	-0.26071300	2.42734600	1.33753400
Si	-1.87316900	1.33216000	-0.97001300	Si	-3.42548400	-0.45630500	-0.62421200
Si	-2.22696500	-1.21968200	1.25623000	Si	-2.03072500	1.20228600	0.21814200
B	-0.00018200	2.18293600	1.32656200	Si	-0.61942700	-2.20394500	1.58271900
11C			11D				
	X	Y	Z		X	Y	Z
B	0.88647200	-0.85170100	0.32406300	B	-0.46561100	-0.62466600	0.85635800
B	0.48992500	0.88905200	0.37637100	B	0.83516300	0.55549500	0.24619700
B	-0.99273200	1.09619900	-0.75810100	B	-0.83449400	0.82475500	-0.05027800
Si	-1.57056900	-0.50545300	-2.04318000	Si	1.64756100	-1.41209600	-1.70537100
Si	-1.68871900	-1.22262900	0.43214000	Si	-2.31861800	-1.97442800	0.41758100
Si	2.57224900	0.25347600	0.99270900	Si	0.36492200	2.54688000	-0.00388500
Si	0.47990000	-0.14048500	2.28648400	Si	0.14146300	-2.44932800	0.01037800
Si	2.23467300	-0.79053700	-1.38586500	B	-0.12232700	-0.51208200	-0.95878300
B	0.33437500	0.06806600	-1.17121500	Si	1.26819900	0.95981900	-1.82550600
Si	0.21851800	-2.19329000	-1.16965400	Si	2.04079300	1.24998700	1.74166600
Si	-0.18149200	2.86405400	-0.31984000	Si	-2.42115600	0.18773300	1.26910300
Si	-1.29017100	1.54677100	1.40972500	Si	-2.28179100	-0.14311500	-1.29839300
Si	-2.98540900	0.52515600	-0.16894400	Si	1.32826800	-1.07502100	1.73927700
Si	1.95207600	1.73499000	-0.93324800	Si	-2.49111700	2.03261100	-0.26910800
Si	0.00250200	-2.50120200	1.33856100	Si	2.93121500	-0.01000700	-0.10913100

B₄Si₁₂

12A				12B			
	X	Y	Z		X	Y	Z
B	0.91296700	-0.79009600	0.49679200	Si	-2.29443000	0.82553300	-0.93740000
B	-1.56606300	0.47180700	-0.35257200	Si	-3.03971600	-0.29959300	1.03524500
B	0.14172700	0.84572300	0.24827900	Si	-1.24268900	1.26045400	1.57276900
Si	1.68587000	0.18586700	-1.43252000	Si	-1.94754000	-2.35022000	0.05002500
Si	-0.66724200	-2.08154400	0.90965800	Si	-0.87924500	2.64944800	-0.40554300
Si	-2.67436300	-0.66021400	1.15630500	Si	0.35313700	-2.11267100	0.64183600
Si	1.48665600	2.35479800	-0.59115200	Si	1.93886300	1.43979900	1.61380600
Si	2.29093600	0.81173700	1.18135500	Si	-0.92173100	-0.94002400	-1.76872400
Si	-2.29596800	-1.32456700	-1.12045500	Si	1.57369400	2.09954300	-0.96500100
Si	0.32405800	0.03979200	2.32917700	Si	1.38307400	-0.04566500	-2.15435400
Si	-1.30899900	0.39342600	-2.40396200	Si	2.33328800	-1.75974200	-0.69636100
Si	-1.02313100	2.50949500	-0.61135100	Si	2.35217600	-0.87884100	1.63262000
Si	-1.56725800	1.48446900	1.53664500	B	0.39188600	0.00777100	1.18767200
Si	0.99242600	-2.49132800	-0.75126200	B	1.70427600	0.20328500	-0.04340100
Si	3.00353700	-1.18601900	-0.02888400	B	0.00164100	0.65343800	-0.49945900
B	-0.17889300	-0.62798200	-0.87844800	B	-1.00267500	-0.55095500	0.42221500
12C				12D			
	X	Y	Z		X	Y	Z
B	-0.03478500	0.41459100	1.21321500	B	1.00182200	-0.42416800	0.09753300
B	-1.12784500	0.44510900	-1.26624600	B	-0.79546200	-0.52659200	0.08527000
B	0.94822300	-0.69238700	0.23873300	B	0.12102500	1.00268000	-0.12732100
Si	2.50101800	0.55557800	-1.16499900	Si	-1.52458700	1.02418100	-1.51627900
Si	2.03899200	0.79094100	1.43522500	Si	0.30247600	-2.21751300	-0.92434100
Si	-2.64555100	-0.13053000	0.49580700	Si	-3.04997000	-0.46987200	0.00769400
Si	-0.86176100	-1.64453100	1.09015600	Si	1.84035200	1.16277900	-1.43709500
Si	-0.91211300	2.09594200	0.20172100	Si	2.52774200	-0.91218600	1.36087900
B	0.43402900	0.81067000	-0.48590800	Si	-1.60681700	1.38966300	1.04432500
Si	1.75615900	2.54904500	-0.25685700	Si	-1.75163200	-0.72163600	2.07698600
Si	0.50210500	-0.73422800	-1.93949500	Si	0.08636500	2.98535500	0.51811300
Si	0.79690900	-2.63255600	-0.36394600	Si	0.27912600	-1.96585400	1.47742600
Si	-2.81075800	1.46876200	-1.28820400	Si	1.98917800	1.40155900	0.88743900
Si	-1.98159700	-1.52887900	-1.22033900	Si	2.47023200	-1.16803800	-1.15219900
Si	3.00800900	-1.14896600	0.48706300	B	0.09220000	2.13908200	-1.41954200
Si	-1.46984900	0.01014300	2.63108600	Si	-1.71231500	-1.29093900	-1.85578400

B₄Si₁₃

13A				13B			
	X	Y	Z		X	Y	Z
B	0.66568200	-0.00064200	-1.13207000	Si	-1.43977000	0.30007600	-1.79436500
B	-1.54869900	0.00011700	0.72091000	Si	-3.12710900	-0.12122700	-0.16029400
B	-0.02246300	-0.93318200	0.22223000	Si	-1.86105400	1.76209500	0.50612000
Si	2.09900200	0.00115200	1.04179400	Si	-2.02938100	-1.45389300	1.70133000
Si	-0.69494400	1.42130100	-1.95884400	Si	-0.52368000	2.50928800	-1.35834100
Si	-2.83433700	-0.00056500	-1.07008500	Si	-0.50478100	0.61386900	2.16828800
Si	1.29987100	-2.14224200	1.44255800	Si	1.95156300	1.75851800	-1.04994600
Si	1.46187900	-1.99074900	-1.09375300	Si	-0.49440500	-2.44491200	0.02177400
Si	-2.03815500	1.96193400	0.08112800	Si	2.21268100	-0.77688700	-1.71253700
Si	-0.69364800	-1.42436100	-1.95817300	Si	1.88446600	-1.98773900	0.44046300
Si	-0.93131800	1.42409300	2.14527600	Si	1.84602600	-0.36861600	2.28944400
Si	-0.93151800	-1.42272500	2.14629800	Si	1.76560600	1.82627400	1.34073400
Si	-2.03743400	-1.96225400	0.08192000	B	0.13243500	0.95994400	0.06209900
Si	1.46101000	1.98985000	-1.09651600	B	1.71818600	0.09430500	0.19401000
Si	2.87208100	-0.00029200	-1.21267800	B	0.34974700	-0.69071800	-0.59854200
B	-0.02318200	0.93392800	0.22072200	B	-1.06803000	-0.34509900	0.34373700
13C				13D			
	X	Y	Z		X	Y	Z
Si	-0.70789100	-1.99269200	-1.92080500	B	-1.36798400	0.77367900	-0.01908700
Si	2.25808100	0.12516500	-1.18223000	B	-0.46897900	-0.77736700	-0.39458000
Si	1.60927400	-2.20930000	-1.10591400	B	1.15662800	-0.07521300	-0.07484400
Si	-1.43495100	1.96911400	-0.95945700	Si	-2.47691600	-0.39202900	1.53564700
Si	1.83378500	1.93270400	0.74469100	Si	0.92900000	0.96636100	-1.95456800
Si	-1.98355300	-1.62444300	0.16305600	Si	-1.16355200	1.68560600	1.91847300
Si	-3.19933500	0.21434600	-1.00442500	Si	-2.51650600	-0.60568700	-1.09349800
Si	1.28100000	-1.95849700	1.35410000	Si	-0.74503800	-2.18884500	1.32934100
Si	-2.62873100	0.59338500	1.34834400	Si	1.09998400	-1.38720900	-1.76457500
Si	2.92475500	-0.10990900	1.16464200	Si	2.61453300	1.39380500	-0.34033100
Si	-0.51662900	1.73885400	1.31300900	Si	-1.48484300	1.49068700	-2.01704100
Si	1.41063300	2.20672900	-1.68182200	Si	1.52331400	-1.16724100	1.80615700
B	0.74618500	0.07644200	0.99194000	Si	-0.68720200	2.73766500	-0.25071100
B	0.13606700	-0.91018100	-0.33916900	Si	-1.01817900	-2.58806200	-1.09537600
B	0.21436100	0.81658000	-0.56379700	Si	1.29972800	1.20717600	1.86140100
B	-1.14637700	-0.13589600	-1.27349400	B	-0.25087300	-0.08035400	1.12138600

B₄Si₁₄

14A				14B			
	X	Y	Z		X	Y	Z
B	0.69209200	1.34172100	-0.00111200	B	0.10181000	-0.43219100	0.90064600
B	0.06418700	-0.21502300	0.87409000	B	-0.07344900	-0.43554400	-0.90872200
B	-1.34109100	-0.75409100	0.00187400	B	0.13851300	1.29221600	-1.56469500
Si	1.73075600	0.59806200	-2.00526700	Si	1.24099800	-2.38413900	1.06989500
Si	-1.96327300	-0.21198300	1.89758600	Si	-1.14421700	2.21315600	-0.10622500
Si	-0.38315200	1.66346800	-1.88944600	Si	2.18618600	-0.26115000	1.78275100
Si	1.73196800	0.60239800	2.00407800	Si	-1.81478000	-1.31278800	0.21203000
Si	1.12588100	-1.74071900	-1.95959200	Si	1.13592100	-2.20567300	-1.60018100
Si	-1.13534400	-2.48623000	1.25034100	Si	-1.64622200	0.55483400	-1.97762900
Si	-2.64882800	1.06062400	-0.00368100	Si	1.03162400	2.90909200	-0.47431000
Si	-0.38153800	1.66689900	1.88752000	Si	-1.48080700	0.60775600	1.97916200
Si	-1.14003800	-2.49454100	-1.23316400	Si	1.77401500	0.11298700	-2.13536700
Si	-0.94249100	2.96682800	-0.00238800	Si	0.60823100	1.65376100	1.68035700
Si	2.17478300	-1.10818500	-0.00399500	Si	-1.22301700	-1.88235800	-1.95978800
Si	-1.96135200	-0.22147800	-1.89808500	Si	2.69462800	1.06818200	-0.16044600
B	0.06259200	-0.21682700	-0.87390900	B	1.47123900	-0.66506900	-0.16392700
Si	1.13467400	-1.73588400	1.95767900	Si	-3.10608700	0.85266200	0.05622400
14C				14D			
	X	Y	Z		X	Y	Z
B	1.74484100	0.08819300	-0.00574800	Si	-1.83174500	2.01977300	0.56383000
B	-1.10284100	1.08165700	0.00505400	Si	-3.31200600	0.08596700	0.36541700
B	0.09394400	0.10989400	-0.89074300	Si	-0.00189400	-0.70734800	2.62680400
Si	0.37458500	-2.03985300	-0.02053800	Si	-2.48294800	-0.46418200	-2.02294800
Si	1.65618300	1.63717500	1.37600000	Si	-0.00121500	1.75205300	2.09525600
Si	-0.23141100	3.08643300	-0.01728600	Si	-1.18521800	-2.19101700	-0.88664300
Si	-0.74375700	-1.51453000	-2.07846100	Si	1.82872600	-1.56749700	1.36364200
Si	1.81136000	-0.71921200	-2.00744200	Si	-1.19420500	1.59819000	-1.72937800
Si	-0.77682200	1.83409500	1.94406400	Si	1.82875400	2.01883300	0.56592300
Si	1.64784200	1.63753500	-1.38480200	Si	1.19509800	1.59874500	-1.72909300
Si	-2.46830400	-0.00674400	1.26809500	Si	2.48289900	-0.46576200	-2.02393000
Si	-2.52043100	-0.00404000	-1.20357500	Si	1.19159200	-2.19257700	-0.87740600
Si	-0.80203600	1.79179500	-1.95038300	B	-0.00026500	-0.81054800	0.42677500
Si	1.81374000	-0.71838900	2.00054200	B	1.40927500	-0.05498800	-0.27720200
Si	2.76256700	-1.77795000	-0.00570800	B	-0.00017000	0.92477400	0.03677000
B	0.09447100	0.11210000	0.89817900	B	-1.41294900	-0.05371400	-0.27294000
Si	-0.70301500	-1.54328900	2.07231700	Si	3.31001400	0.08992100	0.36257300

B₄Si₁₅

15A				15B			
	X	Y	Z		X	Y	Z
B	-0.34128100	0.33481400	0.98539400	B	-1.46468600	0.66510100	-0.11814500
B	1.31887500	0.31973600	0.35717100	B	-0.10853500	-0.26678000	-0.84565700
B	0.08848700	-0.68789600	-0.50163700	B	1.32505200	-0.02830400	0.26171500
Si	-1.22590400	2.37157800	0.41302700	Si	-2.50125400	-0.86034000	1.36859900
Si	1.94099400	-1.63531500	1.11482300	Si	1.47254900	0.80438400	-1.85687500
Si	-2.64612800	0.69009600	1.15782000	Si	-1.44377900	1.20237900	1.93002500
Si	1.01521900	2.21375500	1.38073700	Si	-2.00119700	-0.39557300	-2.05932900
Si	-0.72303100	2.13162000	-1.88902300	Si	-0.85181600	-2.51164000	1.04494200
Si	1.92719500	-0.01591300	-1.60748700	Si	1.45825600	-1.58250000	-1.69616900
Si	-3.09300500	-0.74140700	-0.73535900	Si	1.56001600	2.11539300	0.52176700
Si	1.04142700	0.03205800	2.59296200	Si	-0.72854100	1.64587100	-1.88972900
Si	-1.26090800	-0.17508300	-2.35512500	Si	1.18149100	-1.57487300	1.94532500
Si	-1.29049200	-0.68819200	2.65358800	Si	-0.78249200	2.84286400	0.18441200
Si	1.54652000	2.23380700	-1.05570200	Si	-0.72963400	-2.31024100	-1.37740300
Si	-1.49414200	-1.85446900	0.62360100	Si	0.86030900	0.76114600	2.34054000
B	-1.32284100	0.45241900	-0.47444000	B	-0.39255600	-0.40255500	0.87944400
Si	0.53926000	-1.79296300	-2.43077400	Si	2.85692200	-1.43541700	0.24976300
Si	0.36682700	-2.83307500	-0.26439400	Si	3.40958900	0.92813400	-0.38928500
15C				15D			
	X	Y	Z		X	Y	Z
B	1.38634100	0.42263100	-0.18729800	B	-1.36475800	0.79750800	-0.56766100
B	0.00036800	0.60760600	0.94457600	B	0.21596400	-1.38199200	0.42481400
B	-1.38727400	0.41460300	-0.18635800	B	0.03531500	-0.24360500	-0.96592100
Si	1.61767900	-2.17244700	0.11837000	Si	1.18371800	1.53568900	-1.11646100
Si	-1.19283500	2.42166400	0.45523800	Si	-1.87257200	1.29892700	1.33057300
Si	1.55037900	-0.39804500	-2.03730000	Si	-1.61779600	-2.61017100	0.28051900
Si	2.07228600	0.68703100	1.81623600	Si	1.90876200	-0.44823700	-2.10059700
Si	0.00200400	-1.87555000	1.71387100	Si	-1.83760600	-0.54174300	-2.02455300
Si	-2.07013700	0.67680200	1.81987000	Si	-1.20436200	-1.21892600	2.02922800
Si	-1.20962700	1.94546200	-1.88859200	Si	-3.08075300	-0.52131000	0.11701400
Si	1.18547200	2.42833900	0.45164600	Si	1.72288500	-0.70865400	1.82746500
Si	-1.61627000	-2.16828800	0.11874600	Si	2.24853500	-1.97944700	-0.07658200
Si	1.20465100	1.94674000	-1.89115000	Si	0.07548300	-2.23447000	-1.52198600
Si	0.00352500	0.06545600	3.04426600	Si	-0.85994800	2.90725600	-0.33901000
Si	-1.54711400	-0.39886000	-2.03939700	Si	-0.93335500	1.79891700	-2.41652900
B	0.00363600	-0.71878900	-0.27841100	B	-0.01949100	0.36955500	0.64796800
Si	-3.29259700	-0.51089900	0.02113600	Si	1.49812100	1.77165900	1.25552400
Si	3.29031300	-0.50864400	0.02035500	Si	3.24310200	0.33860700	-0.00553400

Table S3. CCSD(T)//aug-cc-pVTZ energies for isomers of $B_4Si_{4-15}^-$ clusters.

$B_4Si_4^-$	4A	4B
	-1255.363026	-1255.349767
	4C	4D
	-1255.348797	-1255.347817

$B_4Si_5^-$	5A	5B
	-1544.453834	-1544.43737
	5C	5D
	-1544.437206	-1544.428984

$B_4Si_6^-$	6A	6B
	-1833.572431	-1833.570003
	6C	6D
	-1833.560286	-1833.556028

$B_4Si_7^-$	7A	7B
	-2123.076171	-2123.073
	7C	7D
	-2123.070498	-2123.060494

$B_4Si_8^-$	8A	8B
	-2412.405737	-2412.399061
	8C	8D
	-2412.398203	-2412.397372

$B_4Si_9^-$	9A	9B
	-2701.802517	-2701.789986
	9C	9D
	-2701.788043	-2701.78398

$B_4Si_{10}^-$	10A	10B
	-2991.205087	-2991.196577
	10C	10D
	-2991.192546	-2991.189681

$B_4Si_{11}^-$	11A	11B
	-3280.608385	-3280.602256
	11C	11D
	-3280.601042	-3280.596903

$B_4Si_{12}^-$	12A	12B
	-3570.021515	-3570.008228
	12C	12D
	-3570.000514	-3569.998054

$B_4Si_{13}^-$	13A	13B
	-3859.446024	-3859.43699
	13C	13D
	-3859.435012	-3859.43301

$B_4Si_{14}^-$	14A	14B
	-4148.868494	-4148.858985
	14C	14D
	-4148.856019	-4148.855177

$B_4Si_{15}^-$	15A	15B
	-4438.267423	-4438.258951
	15C	15D
	-4438.257888	-4438.254909

Table S4. CCSD(T)//aug-cc-pVTZ energies for isomers of B₄Si₄₋₁₅ clusters.

B ₄ Si ₄	4A'	4B'
	-1255.285248	-1255.26716
	4C'	4D'
	-1255.260468	-1255.259624

B ₄ Si ₅	5A'	5B'
	-1544.370823	-1544.366475
	5C'	5D'
	-1544.356274	-1544.351542

B ₄ Si ₆	6A'	6B'
	-1833.439035	-1833.431593
	6C'	6D'
	-1833.427173	-1833.422529

B ₄ Si ₇	7A'	7B'
	-2123.076171	-2123.070102
	7C'	7D'
	-2123.069	-2123.06499

B ₄ Si ₈	8A'	8B'
	-2412.31302	-2412.306497
	8C'	8D'
	-2412.30051	-2412.297182

B ₄ Si ₉	9A'	9B'
	-2701.713433	-2701.708604
	9C'	9D'
	-2701.702964	-2701.702988

B ₄ Si ₁₀	10A'	10B'
	-	-2991.112842
	2991.119779	
	10C'	10D'
-	-2991.105297	
2991.110006		

B ₄ Si ₁₁	11A'	11B'
	-3280.522803	-3280.506601
	11C'	11D'
	-3280.505003	-3280.500387

B ₄ Si ₁₂	12A'	12B'
	-3569.927677	-3569.924973
	12C'	12D'
	-3569.914993	-3569.912658

B_4Si_{13}	13A'	13B'
	-3859.34235	-3859.332123
	13C'	13D'
	-3859.330703	-3859.327823

B_4Si_{14}	14A'	14B'
	-4148.772431	-4148.763099
	14C'	14D'
	-4148.760012	-4148.758003

B_4Si_{15}	15A'	15B'
	-4438.174449	-4438.163963
	15C'	15D'
	-4438.161983	-4438.160131