

Supporting Information

Analysis of the electronic delocalization in some B_{12} 's isoelectronic analogues doped with beryllium and/or carbon

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Content:

Section 1. Global minimum Cartesian coordinates:

B_{12} SI3

$B_{11}C^+$ SI3

$B_{11}Be^-$ SI4

$B_{10}C_2^{+2}$ SI4

$B_{10}Be_2^{-2}$ SI5

$B_{10}BeC$ SI5

$B_9C_2Be^+$ SI6

$B_9CBe_2^-$ SI6

C_6B_6 SI7

Section 1. Global minimum's Cartesian coordinates (in Å).

B₁₂

B	0.841237000	0.485689000	0.389523000
B	0.000000000	2.016474000	-0.039823000
B	-0.841237000	0.485689000	0.389523000
B	1.600297000	1.820166000	-0.174850000
B	1.746318000	-1.008237000	-0.039823000
B	2.376459000	0.475815000	-0.174850000
B	0.776162000	-2.295981000	-0.174850000
B	-0.776162000	-2.295981000	-0.174850000
B	-2.376459000	0.475815000	-0.174850000
B	-1.600297000	1.820166000	-0.174850000
B	-1.746318000	-1.008237000	-0.039823000
B	0.000000000	-0.971377000	0.389523000

B₁₁C⁺

B	-0.102363000	2.323147000	-0.275318000
B	-1.434534000	1.413680000	-0.030999000
B	-2.430422000	0.177793000	-0.172262000
B	-2.025345000	-1.315556000	-0.251721000
B	-0.522004000	-1.939124000	-0.086011000
B	1.068498000	-2.169022000	-0.230846000
B	2.148827000	-1.063460000	-0.187970000
B	1.908001000	0.510132000	-0.051807000
C	1.226699000	1.821993000	-0.176567000
B	0.234856000	0.885582000	0.493837000
B	0.658098000	-0.749413000	0.506700000
B	-0.975651000	-0.260151000	0.498277000

$B_{11}Be^-$

B	1.800340000	-1.870529000	-0.055809000
B	2.456071000	-0.447513000	-0.047591000
B	1.746496000	1.005279000	-0.010191000
B	0.838989000	-0.536855000	0.121825000
Be	0.002031000	-2.326614000	-0.025545000
B	-1.797089000	-1.873549000	-0.056072000
B	-0.838000000	-0.538296000	0.121319000
B	-2.455241000	-0.451631000	-0.047527000
B	-1.748201000	1.002333000	-0.010055000
B	-0.779291000	2.323724000	-0.054249000
B	-0.000873000	0.923375000	0.113684000
B	0.775174000	2.324953000	-0.054899000

 $B_{10}C_2^{+2}$

B	1.022410000	-1.738153000	-0.071646000
B	-0.505741000	-2.274952000	-0.331912000
C	-1.636000000	-1.427286000	-0.163825000
B	-1.953508000	0.000088000	-0.067429000
C	-1.635868000	1.427431000	-0.163831000
B	-0.505533000	2.274998000	-0.331908000
B	1.022567000	1.738054000	-0.071648000
B	2.316813000	0.775594000	-0.233133000
B	2.316730000	-0.775796000	-0.233135000
B	1.044801000	-0.000039000	0.573429000
B	-0.416186000	-0.852242000	0.580284000
B	-0.416111000	0.852272000	0.580286000

$B_{10}Be_2^{-2}$

Be	-1.150373000	-1.992615000	-0.000119000
B	-2.512761000	-0.780364000	-0.000208000
B	-2.512836000	0.780114000	-0.000052000
Be	-1.150586000	1.992522000	0.000146000
B	-1.038678000	-0.000047000	0.000211000
B	0.439684000	0.864493000	-0.000089000
B	0.439761000	-0.864463000	0.000020000
B	0.623115000	2.511665000	0.000318000
B	0.623374000	-2.511614000	0.000120000
B	1.892094000	-1.612935000	0.000148000
B	1.995079000	0.000100000	-0.000050000
B	1.891935000	1.613126000	-0.000439000

 $B_{10}BeC$

B	0.370671000	-2.217847000	-0.377589000
B	-1.114426000	-1.663420000	-0.040534000
B	-2.340904000	-0.673703000	-0.188655000
B	-2.229250000	0.861351000	-0.259402000
B	-0.893186000	1.762912000	-0.126137000
B	0.599819000	2.304464000	-0.246801000
B	1.876172000	1.442088000	-0.212413000
B	-1.014579000	0.048607000	0.525662000
B	0.487529000	0.872923000	0.552569000
B	1.963774000	-0.141762000	-0.056608000
C	1.591769000	-1.539267000	-0.241882000
Be	0.480320000	-0.935617000	0.900208000

$B_9C_2Be^+$

B	-0.646664000	2.007910000	0.000027000
B	0.944503000	1.767037000	-0.000008000
B	2.401692000	1.222698000	-0.000144000
B	2.861278000	-0.259299000	0.000209000
B	1.175709000	0.009978000	-0.000123000
B	1.989379000	-1.549768000	-0.000036000
B	0.412500000	-1.698963000	0.000023000
C	-1.027524000	-1.805692000	-0.000063000
B	-2.294919000	-1.273667000	-0.000048000
B	-2.701014000	0.268663000	0.000052000
C	-1.906229000	1.414999000	-0.000020000
Be	-0.777452000	-0.032194000	0.000186000

 $B_9CBe_2^-$

C	-0.704454000	2.310537000	0.000000000
B	0.718664000	2.468135000	0.000000000
B	0.000000000	0.965394000	0.000000000
B	2.518942000	-0.628113000	0.000000000
Be	-1.930845000	1.140251000	0.000000000
Be	2.006708000	1.132999000	0.000000000
B	0.877567000	-0.468308000	0.000000000
B	-0.000539000	-2.013751000	0.000000000
B	1.634238000	-1.903721000	0.000000000
B	-1.627225000	-1.905212000	0.000000000
B	-0.844259000	-0.494973000	0.000000000
B	-2.492733000	-0.610697000	0.000000000

C₆B₆

Be	-1.547034000	1.845552000	0.150193000
C	-2.693212000	-0.622567000	-0.014046000
C	-2.693135000	0.622553000	-0.014007000
Be	-1.547072000	-1.845539000	0.150043000
Be	-0.884206000	0.000050000	-0.398508000
C	0.000026000	1.485704000	0.000216000
C	-0.000020000	-1.485617000	0.000282000
C	2.693155000	-0.622597000	0.013663000
C	2.693188000	0.622520000	0.013634000
Be	0.884255000	-0.000005000	0.398483000
Be	1.546991000	-1.845634000	-0.149879000
Be	1.547063000	1.845580000	-0.149947000