Supplementary Material

Dynamical Behavior of Boron Clusters

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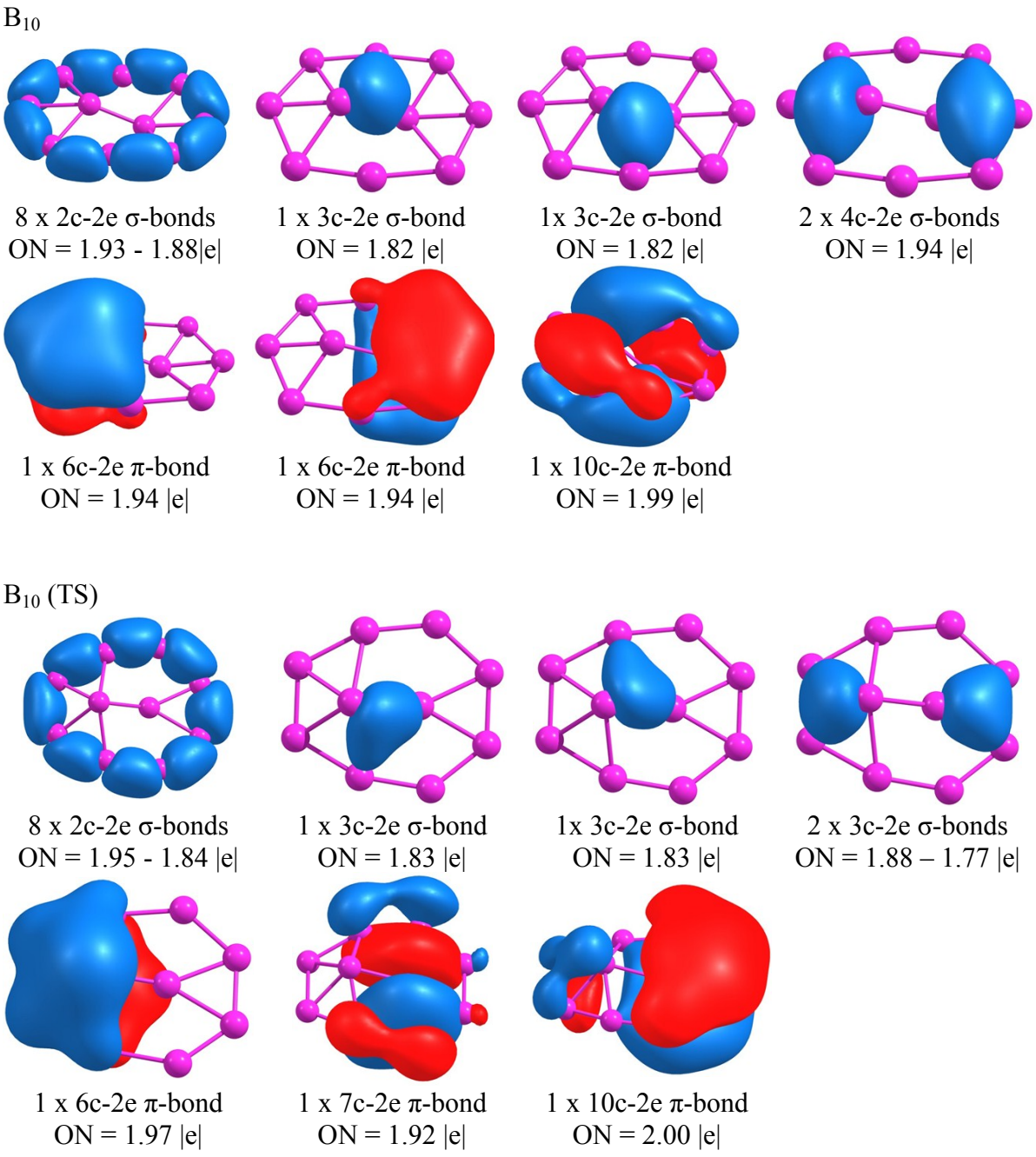
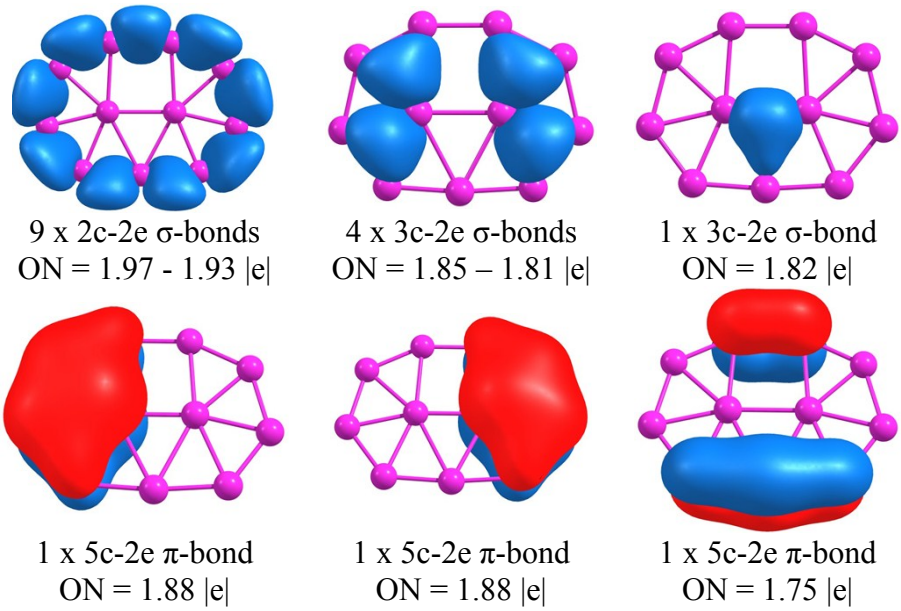


Fig. S1 Adaptive natural density partitioning analysis of the B_{10} and B_{10}(TS) boron clusters.

B_{11}^-



B_{11}^- (TS)

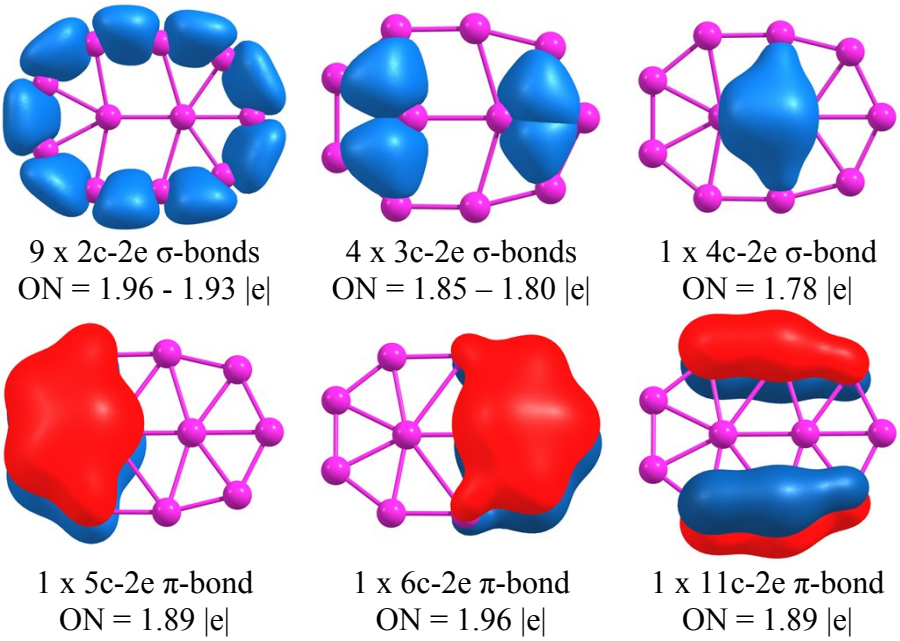


Fig. S2 Adaptive natural density partitioning analysis of the B_{11}^- and B_{11}^-(TS) boron clusters.

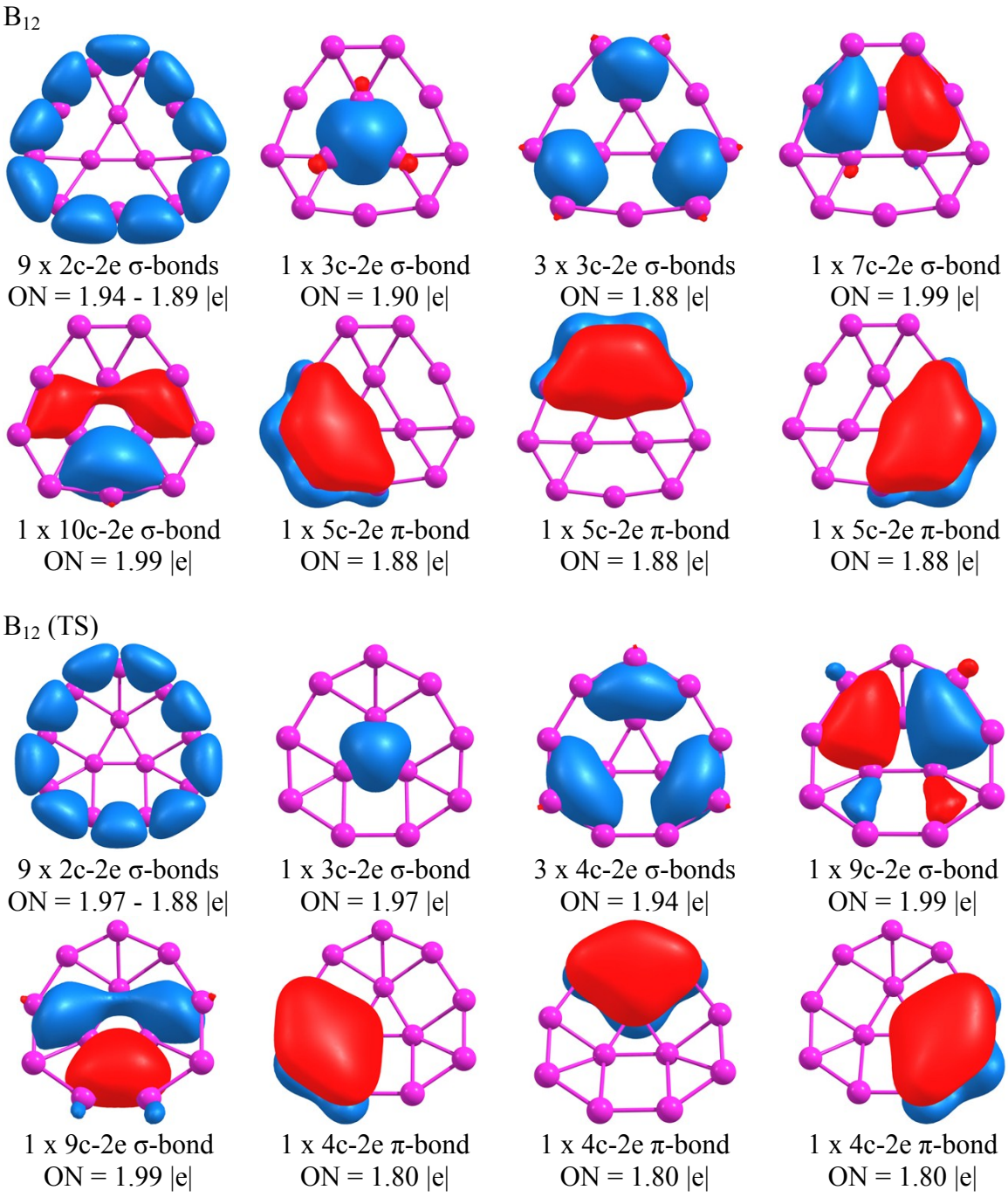
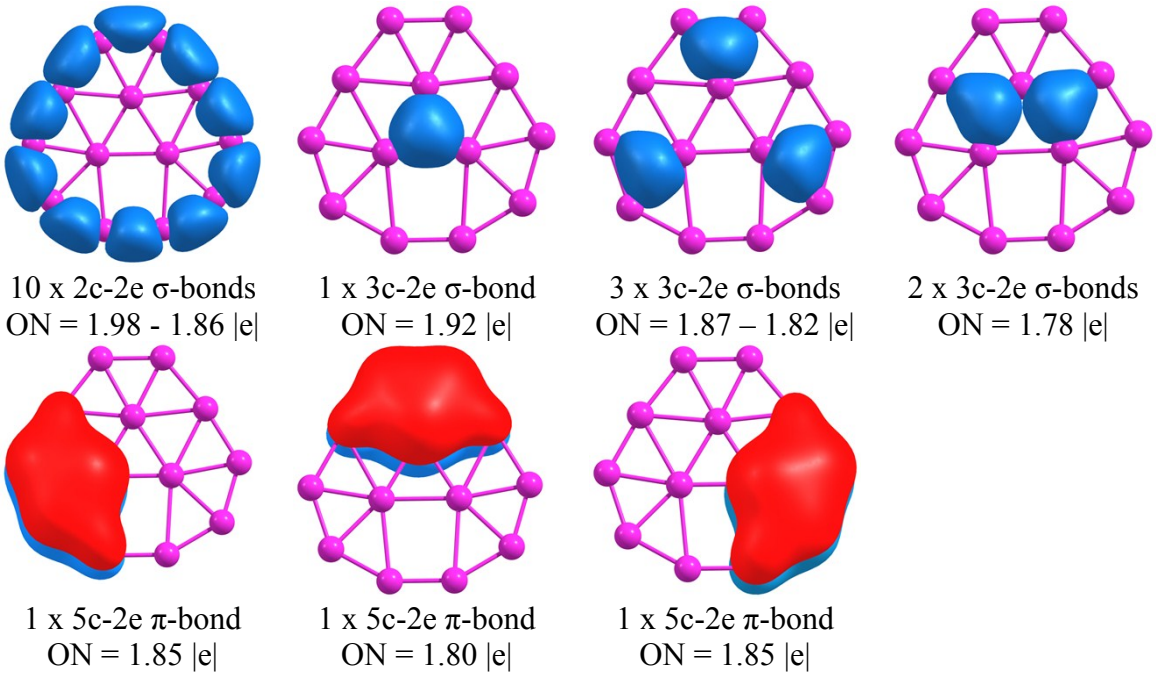


Fig. S3 Adaptive natural density partitioning analysis of the B_{12} and B_{12}(TS) boron clusters.

B_{13}^+



B_{13}^+ (TS)

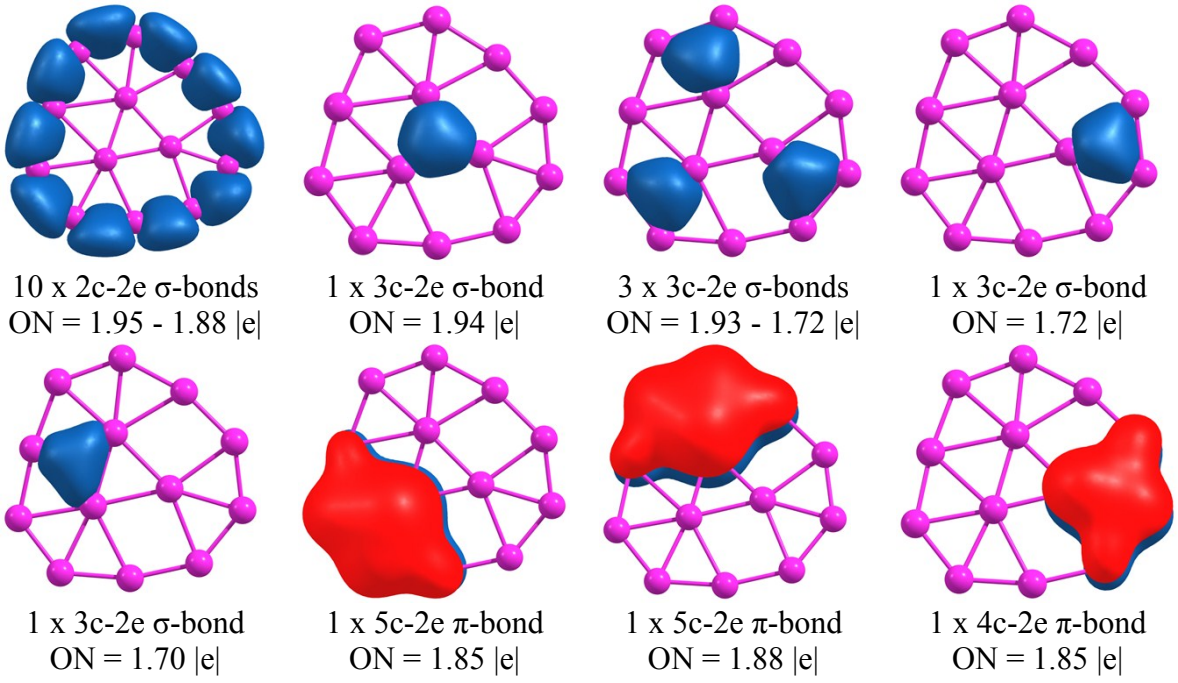


Fig. S4 Adaptive natural density partitioning analysis of the B_{13}^+ and B_{13}^+(TS) boron clusters.

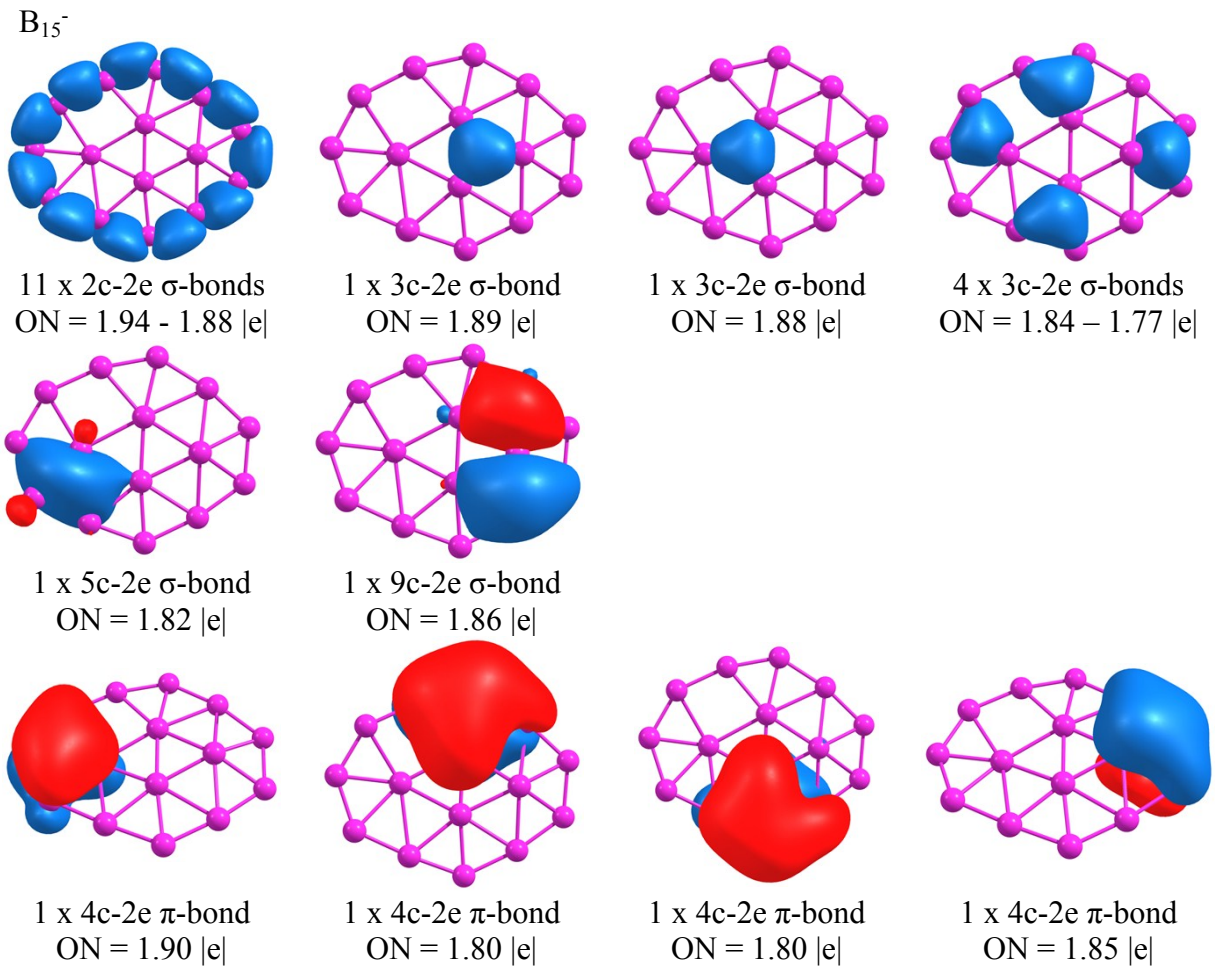


Fig. S5 Adaptive natural density partitioning analysis of the B_{15}^- boron clusters.

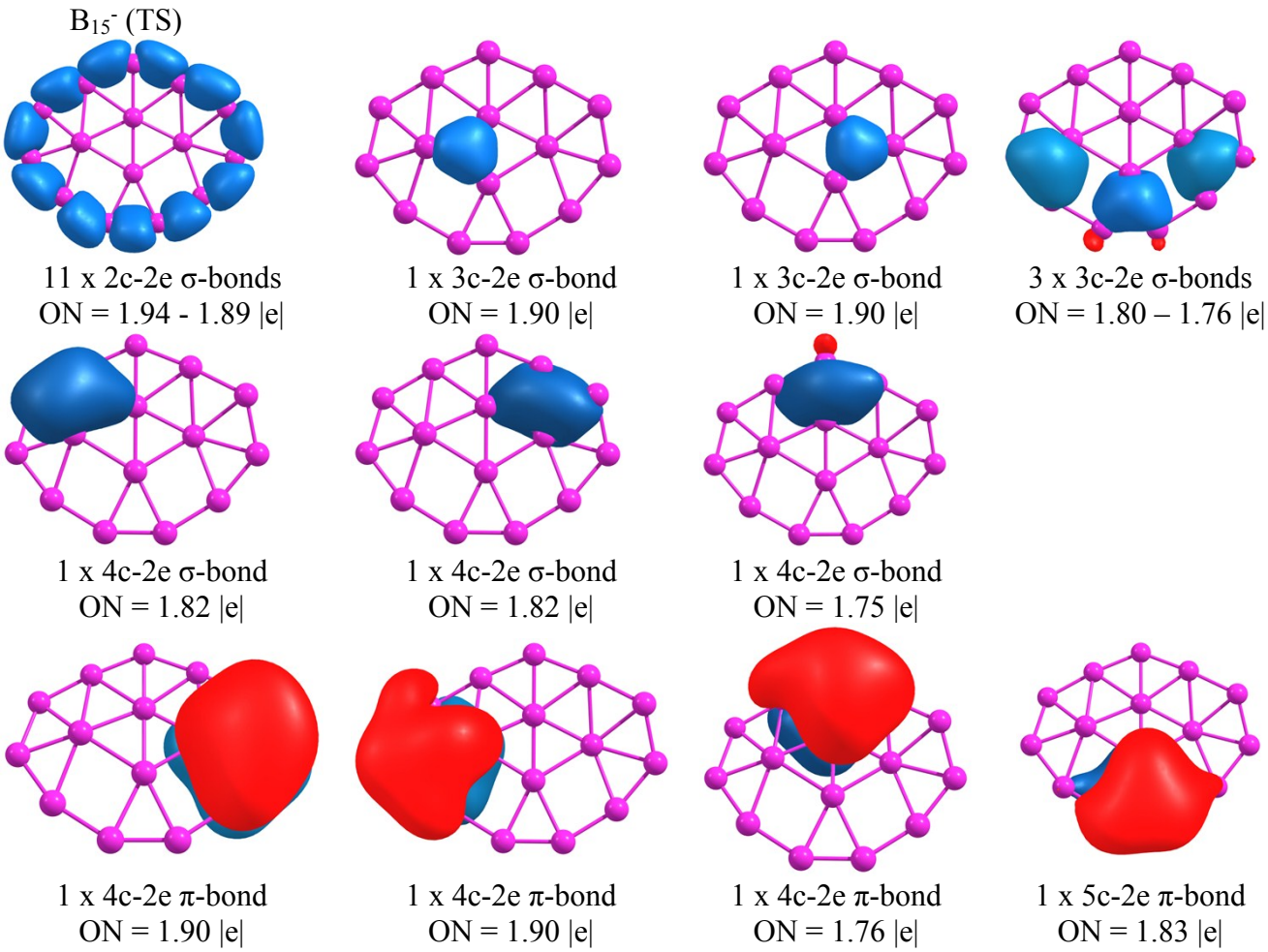


Fig. S6 Adaptive natural density partitioning analysis of the B_{15}^- (TS) boron clusters.

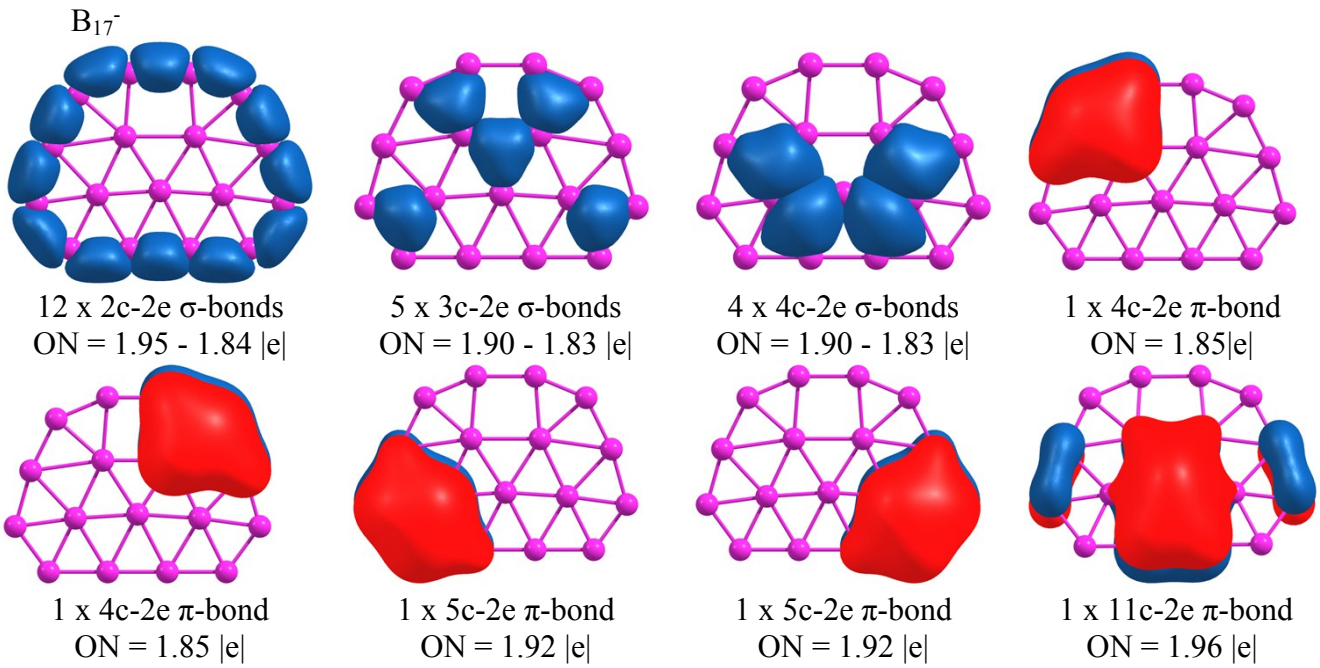


Fig. S7 Adaptive natural density partitioning analysis of the B_{17}^- boron clusters.

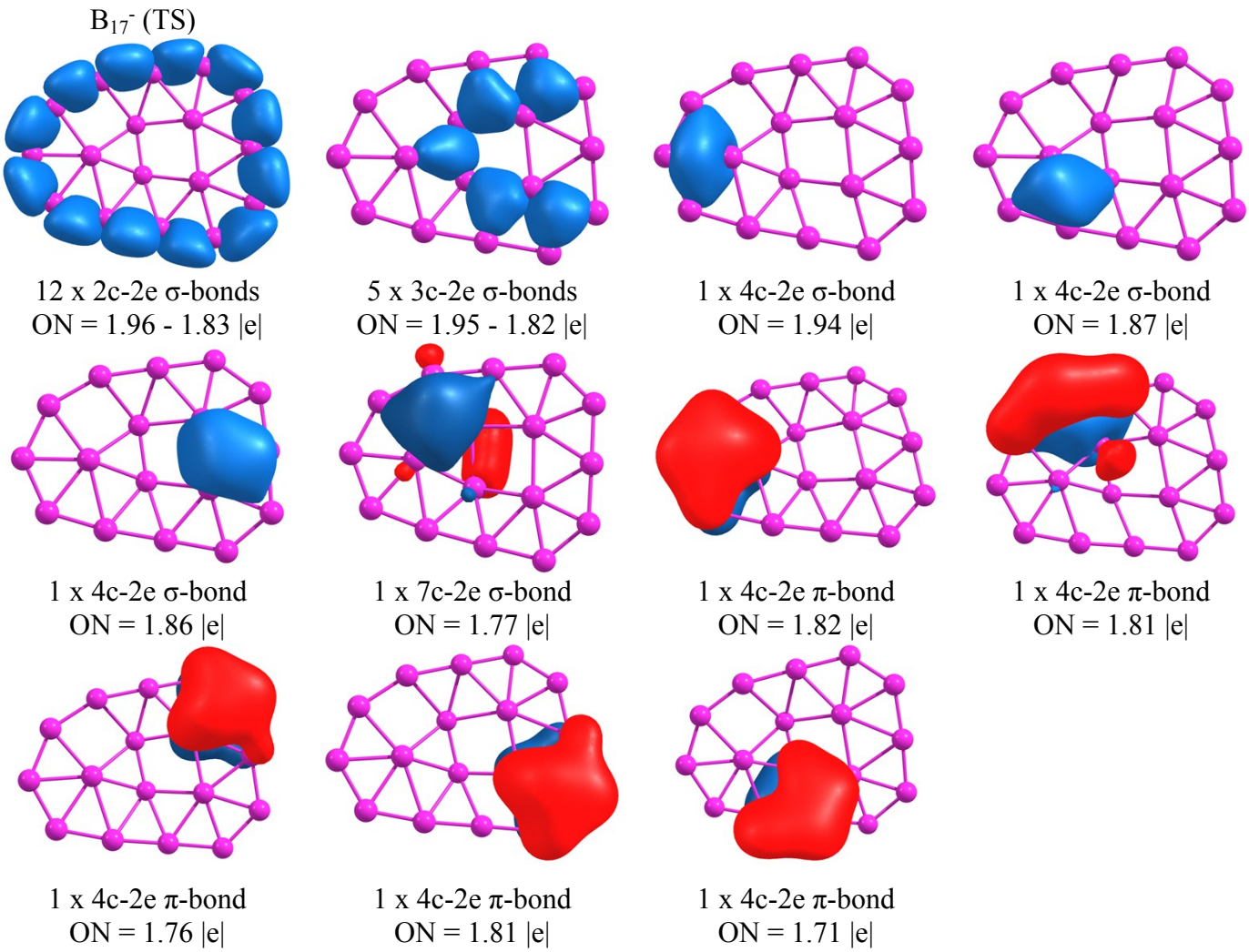


Fig. S8 Adaptive natural density partitioning analysis of the B_{17}^-(TS) boron clusters.

B_{19}^-

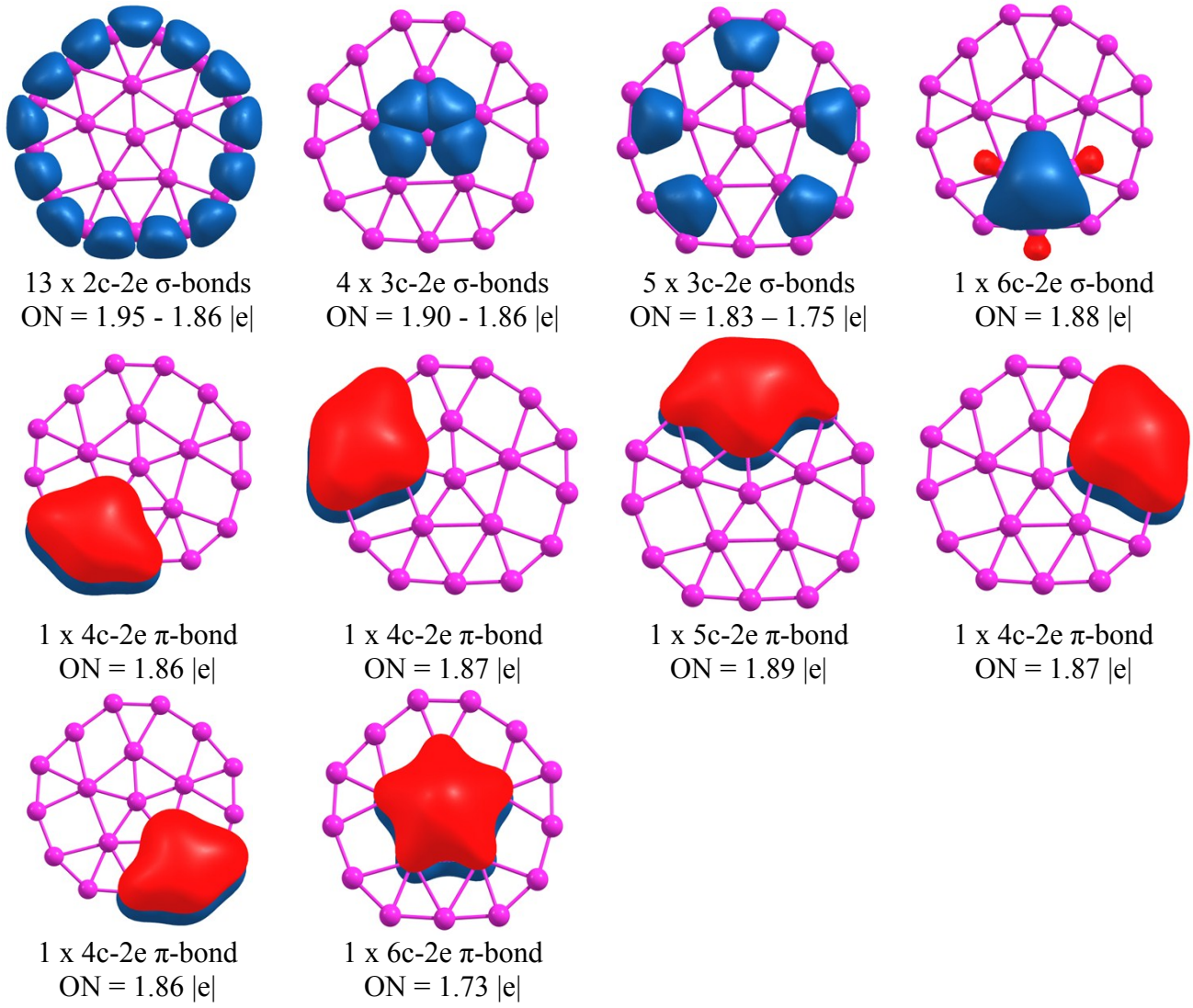


Fig. S9 Adaptive natural density partitioning analysis of the B_{19}^- boron clusters.

B_{19}^- (TS)

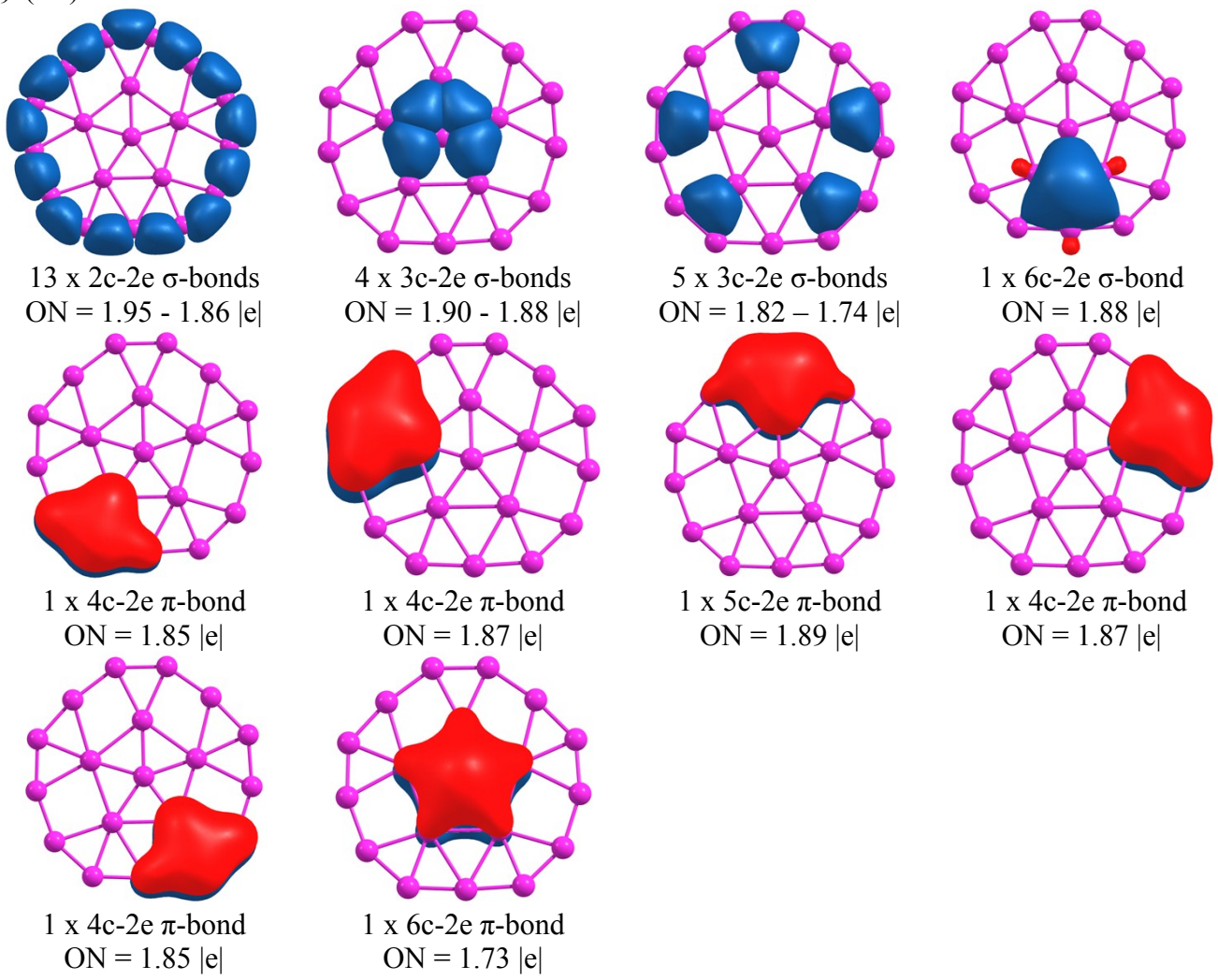


Fig. S10 Adaptive natural density partitioning analysis of the B_{19}^-(TS) boron clusters.

B_{21}^-

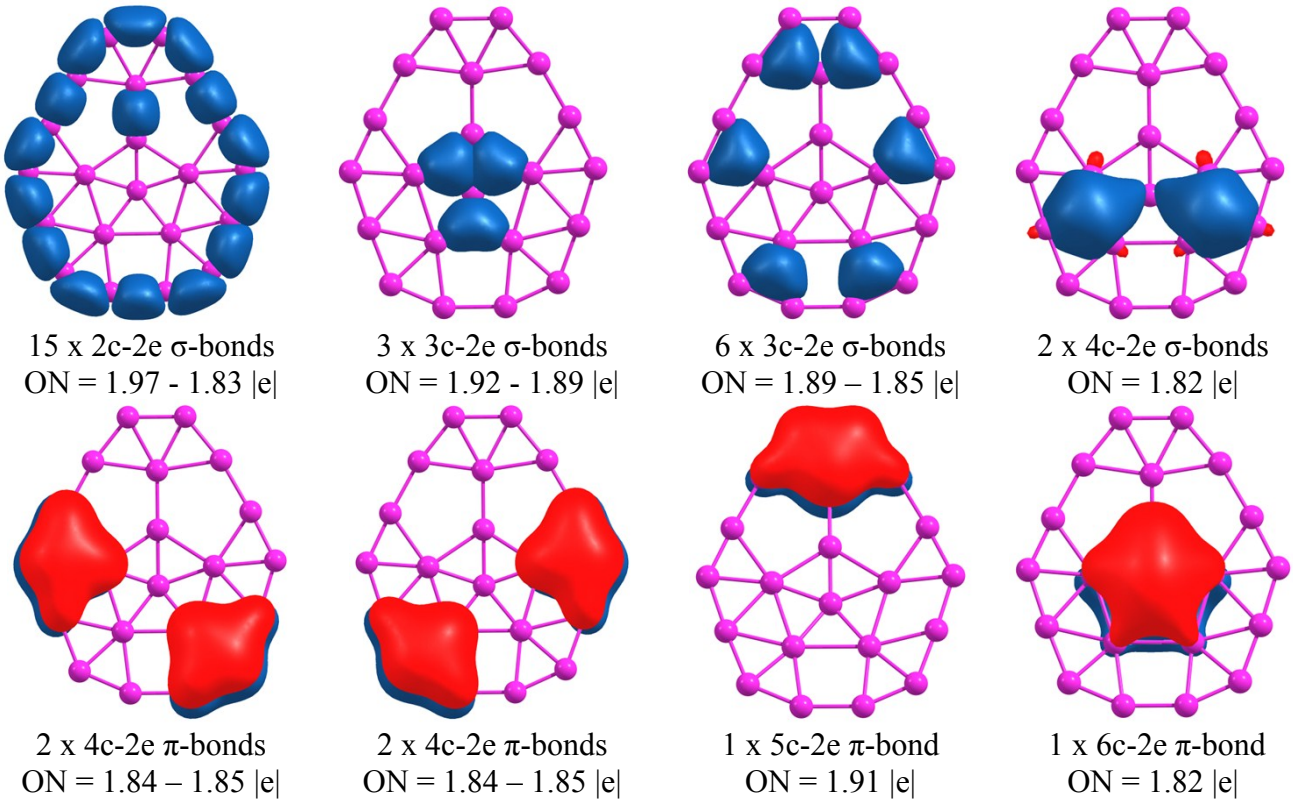


Fig. S11 Adaptive natural density partitioning analysis of the B_{21}^- boron clusters.

B_{21}^- (TS)

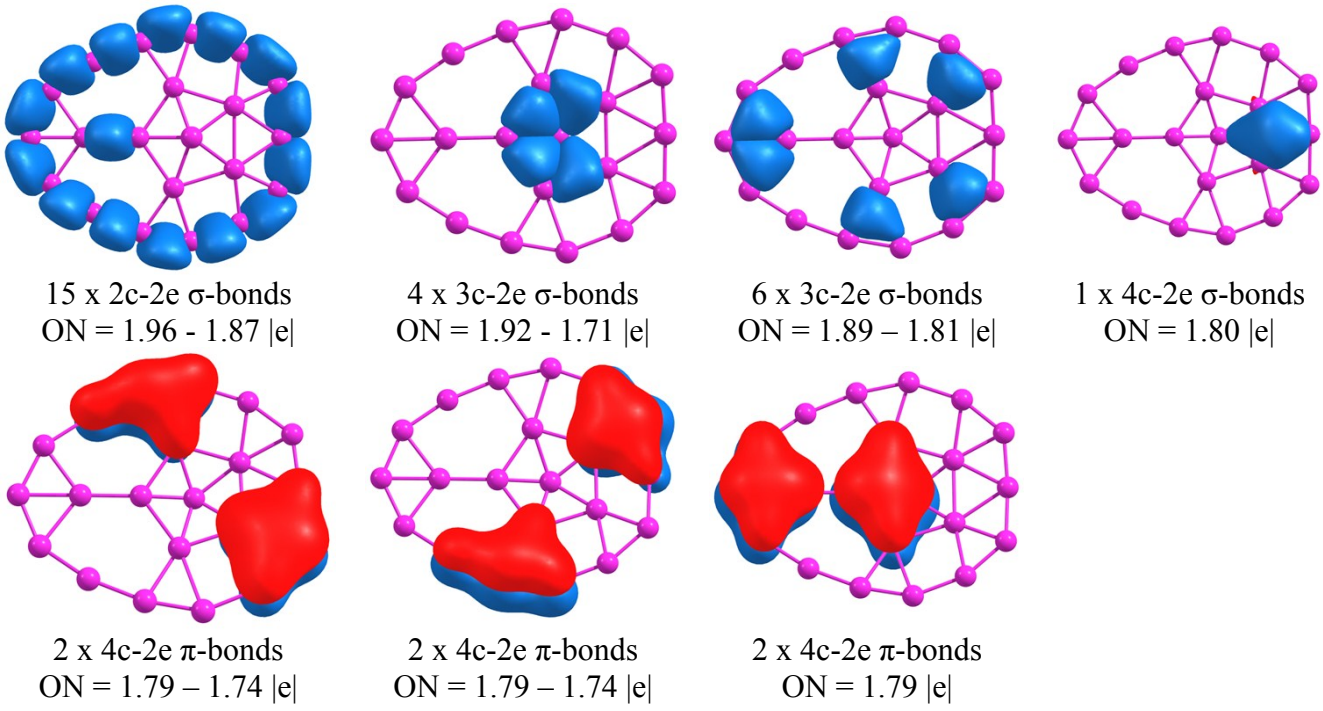


Fig. S12 Adaptive natural density partitioning analysis of the B_{21}^-(TS) boron clusters.

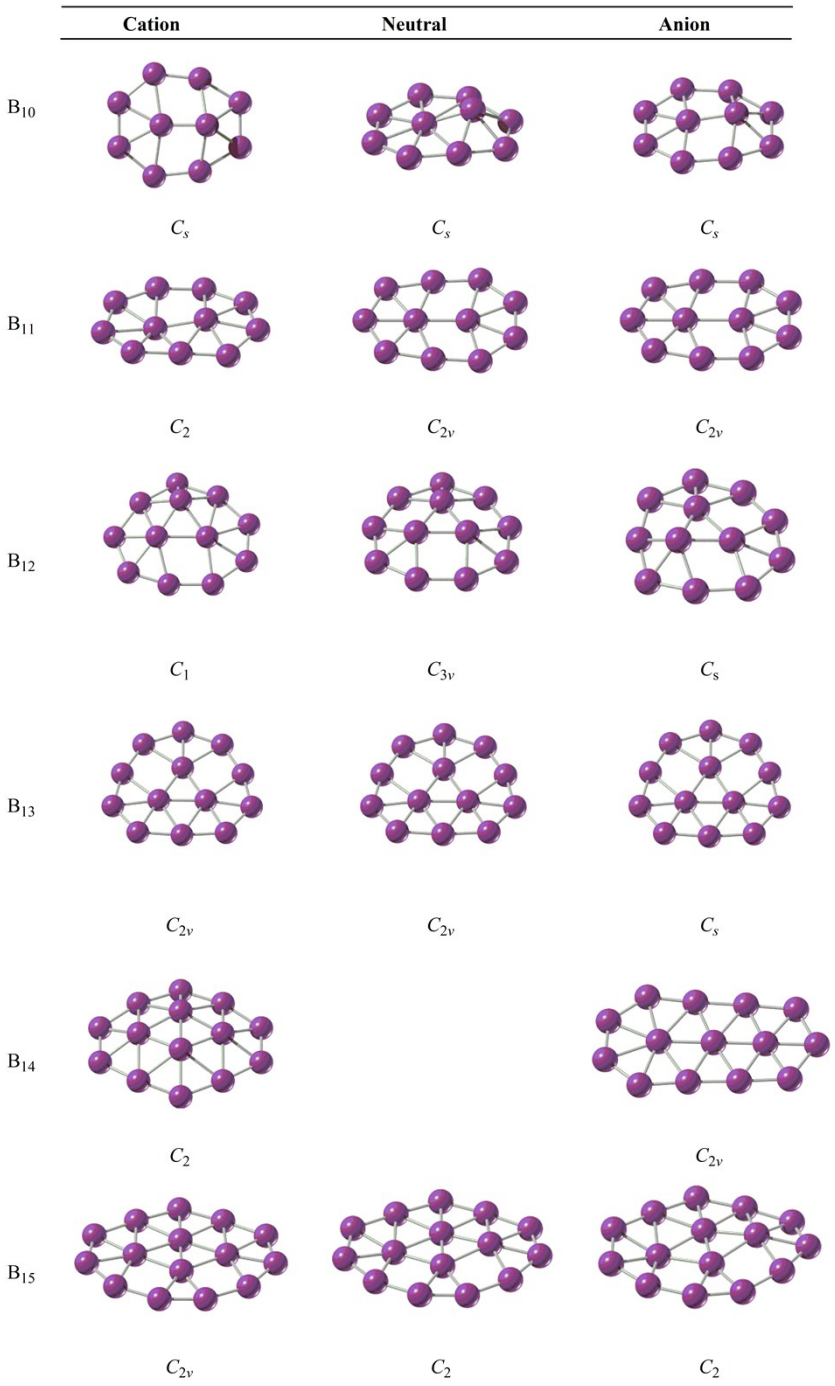


Figure S13. Transition State (**TS**) geometries from B_{10} to B_{15}. We have accepted an arbitrary cut-off of the B—B bond lengths of 1.99 Å (which is somewhat above the typical B—B bond distances in boron wheels) so that only the shortest contacts in the clusters are shown.

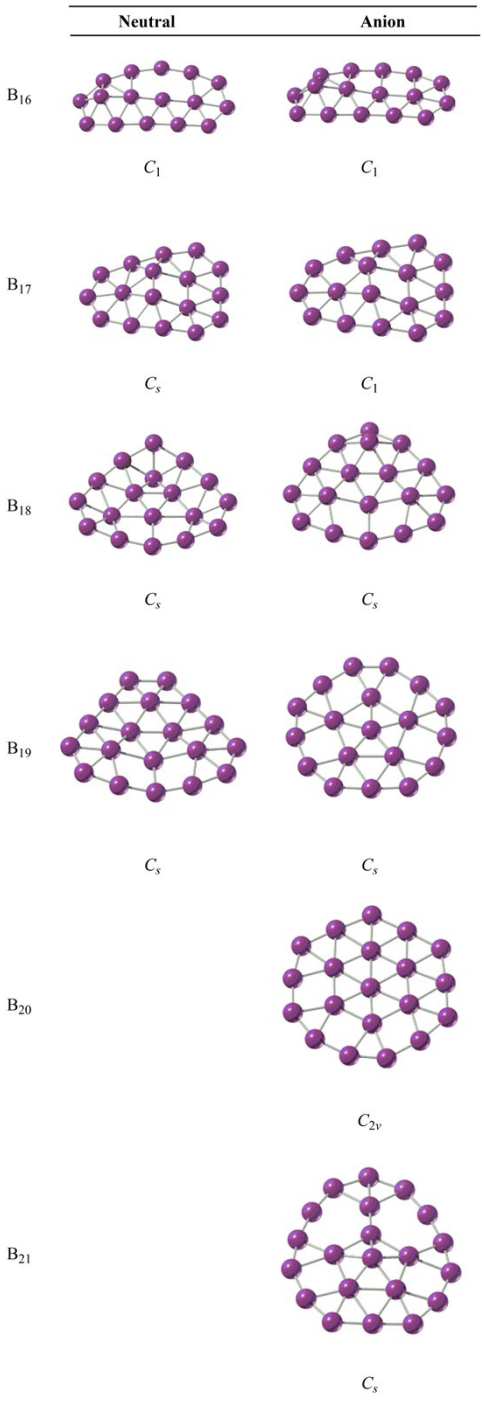


Figure S14. Transition State (**TS**) geometries from B_{16} to B_{21}.We have accepted an arbitrary cut-off of the B—B bond lengths of 1.99 Å (which is somewhat above the typical B—B bond distances in boron wheels) so that only the shortest contacts in the clusters are shown.

Cartesian Coordinates of Optimized Structures

B_{10}^-
E_{zpe}=-248.048571
G= -248.080123

B	0.000000000	0.801954000	0.234314000
B	-1.581437000	0.000000000	0.066859000
B	-1.409685000	-1.598054000	-0.073451000
B	0.000000000	-2.344438000	-0.154269000
B	0.000000000	-0.801954000	0.234314000
B	1.581437000	0.000000000	0.066859000
B	1.409685000	-1.598054000	-0.073451000
B	1.409685000	1.598054000	-0.073451000
B	-1.409685000	1.598054000	-0.073451000
B	0.000000000	2.344438000	-0.154269000

B_{10}^- (TS)
E_{zpe}= -248.023500
G= -248.054686

B	-0.675464000	0.000001000	0.205964000
B	0.725925000	-1.608213000	0.012368000
B	2.092010000	-0.802687000	-0.237686000
B	2.092011000	0.802683000	-0.237687000
B	0.936768000	0.000000000	0.548983000
B	-0.862488000	1.743789000	-0.013661000
B	0.725930000	1.608213000	0.012365000
B	-2.086100000	0.789898000	-0.138491000
B	-0.862492000	-1.743788000	-0.013663000
B	-2.086101000	-0.789895000	-0.138493000

B_{10}^+
E_{zpe}= -247.637616
G= -247.668334

B	0.000000000	0.807840000	0.446380000
B	-1.539850000	0.000000000	0.111983000
B	-1.368295000	-1.593112000	-0.155569000
B	0.000000000	-2.337480000	-0.247224000
B	0.000000000	-0.807840000	0.446380000
B	1.539850000	0.000000000	0.111983000
B	1.368295000	-1.593112000	-0.155569000
B	1.368295000	1.593112000	-0.155569000
B	-1.368295000	1.593112000	-0.155569000
B	0.000000000	2.337480000	-0.247224000

B_{10}^+ (TS)

E_{zpe}= -247.610361
G= -247.641794

B	0.625671000	0.000014000	0.353514000
B	-0.708380000	1.591578000	-0.050446000
B	-2.089939000	0.767427000	-0.239193000
B	-2.089904000	-0.767498000	-0.239196000
B	-0.961781000	-0.000013000	0.655813000
B	0.876406000	-1.763910000	-0.097689000
B	-0.708305000	-1.591585000	-0.050436000
B	2.089972000	-0.764365000	-0.117343000
B	0.876330000	1.763928000	-0.097686000
B	2.089929000	0.764424000	-0.117338000

B_{10}
E_{zpe}= -247.944791
G= -247.974854

B	-0.337373000	0.740101000	0.000000000
B	0.000000000	0.000000000	1.558384000
B	0.000000000	-1.602979000	1.375024000
B	0.124054000	-2.371320000	0.000000000
B	0.337373000	-0.740101000	0.000000000
B	0.000000000	0.000000000	-1.558384000
B	0.000000000	-1.602979000	-1.375024000
B	0.000000000	1.602979000	-1.375024000
B	0.000000000	1.602979000	1.375024000
B	-0.124054000	2.371320000	0.000000000

B_{10} (TS)
E_{zpe}= -247.924487
G= -247.954917

B	-0.033036000	0.572051000	0.000000000
B	0.198096000	-0.651393000	1.562457000
B	0.198096000	-2.061551000	0.776942000
B	0.198096000	-2.061551000	-0.776942000
B	0.892126000	-0.806489000	0.000000000
B	-0.210586000	0.849220000	-1.764786000
B	0.198096000	-0.651393000	-1.562457000
B	-0.615151000	1.980943000	-0.769521000
B	-0.210586000	0.849220000	1.764786000
B	-0.615151000	1.980943000	0.769521000

B_{11}^-
E_{zpe}= -272.879538
G= -272.911309

B	0.000000000	0.891701000	0.029297000
B	0.000000000	0.000000000	1.715672000

B	0.000000000	-1.563921000	1.617704000
B	0.000000000	-2.514782000	0.410321000
B	0.000000000	-0.891701000	0.029297000
B	0.000000000	-0.788289000	-1.798084000
B	0.000000000	-2.156345000	-1.117073000
B	0.000000000	2.156345000	-1.117073000
B	0.000000000	1.563921000	1.617704000
B	0.000000000	2.514782000	0.410321000
B	0.000000000	0.788289000	-1.798084000

B_{11}^- (TS)
E_{zpe}= -272.878856
G= -272.910011

B	0.000000000	0.000000000	0.909688000
B	0.000000000	1.749796000	-1.192006000
B	0.000000000	0.786159000	-2.371656000
B	0.000000000	-0.786159000	-2.371656000
B	0.000000000	0.000000000	-0.872201000
B	0.000000000	-1.769056000	0.379234000
B	0.000000000	-1.749796000	-1.192006000
B	0.000000000	0.000000000	2.562960000
B	0.000000000	1.769056000	0.379234000
B	0.000000000	1.400660000	1.884205000
B	0.000000000	-1.400660000	1.884205000

B_{11}^+
E_{zpe}= -272.464789
G= -272.497178

B	-0.082150000	0.749139000	0.000000000
B	0.045704000	-0.317000000	1.611835000
B	-0.119209000	-1.878608000	1.349358000
B	-0.053730000	-2.637373000	0.000000000
B	0.308324000	-0.933600000	0.000000000
B	0.045704000	-0.317000000	-1.611835000
B	-0.119209000	-1.878608000	-1.349358000
B	-0.077785000	2.382068000	-0.766871000
B	0.065069000	1.224457000	1.780323000
B	-0.077785000	2.382068000	0.766871000
B	0.065069000	1.224457000	-1.780323000

B_{11}^+ (TS)
E_{zpe}= -272.462957
G= -272.494112

B	0.000000000	0.861590000	0.043490000
B	0.000000000	0.000000000	1.581977000
B	0.429402000	-1.518653000	1.610072000

B	0.523533000	-2.505482000	0.419510000
B	0.000000000	-0.861590000	0.043490000
B	0.194456000	-0.751849000	-1.799970000
B	0.501289000	-2.095195000	-1.064093000
B	-0.501289000	2.095195000	-1.064093000
B	-0.429402000	1.518653000	1.610072000
B	-0.523533000	2.505482000	0.419510000
B	-0.194456000	0.751849000	-1.799970000

B_{11}
E_{zpe}= -272.760377
G= -272.792994

B	0.000000000	0.862533000	0.056543000
B	0.000000000	0.000000000	1.625129000
B	0.000000000	-1.574480000	1.628554000
B	0.000000000	-2.524415000	0.406994000
B	0.000000000	-0.862533000	0.056543000
B	0.000000000	-0.776974000	-1.811510000
B	0.000000000	-2.141515000	-1.093146000
B	0.000000000	2.141515000	-1.093146000
B	0.000000000	1.574480000	1.628554000
B	0.000000000	2.524415000	0.406994000
B	0.000000000	0.776974000	-1.811510000

B_{11} (TS)
E_{zpe}= -272.759473
G= -272.791734

B	0.000000000	0.000000000	0.918359000
B	0.000000000	1.777562000	-1.209660000
B	0.000000000	0.771892000	-2.365209000
B	0.000000000	-0.771892000	-2.365209000
B	0.000000000	0.000000000	-0.804497000
B	0.000000000	-1.689965000	0.339045000
B	0.000000000	-1.777562000	-1.209660000
B	0.000000000	0.000000000	2.588047000
B	0.000000000	1.689965000	0.339045000
B	0.000000000	1.387773000	1.884870000
B	0.000000000	-1.387773000	1.884870000

B_{12}^-
E_{zpe}= -297.686745
G= -297.719905

B	0.152209000	-0.482925000	2.387958000
B	0.132147000	2.308667000	0.798056000
B	0.132147000	2.308667000	-0.798056000

B	0.016573000	1.044927000	-1.761933000
B	-0.289062000	-0.496914000	-0.835137000
B	0.112713000	-1.841671000	-1.623491000
B	0.152209000	-0.482925000	-2.387958000
B	0.043708000	-2.024999000	0.000000000
B	0.016573000	1.044927000	1.761933000
B	0.112713000	-1.841671000	1.623491000
B	-0.289062000	-0.496914000	0.835137000
B	-0.292869000	0.960831000	0.000000000

B_{12}^- (TS)
E_{zpe}= -297.659494
G= -297.692770

B	0.875999000	-0.321472000	0.359990000
B	-0.875610000	-0.321580000	0.359337000
B	-0.783224000	-2.005130000	-0.122565000
B	-2.150651000	-1.211636000	-0.150182000
B	-0.000004000	1.041630000	0.650684000
B	-1.405151000	1.548918000	-0.153633000
B	-2.426837000	0.309514000	-0.092661000
B	0.783160000	-2.004859000	-0.122650000
B	2.426698000	0.309574000	-0.093157000
B	1.404908000	1.549132000	-0.153566000
B	-0.000135000	2.317444000	-0.331599000
B	2.150847000	-1.211535000	-0.150000000

B_{12}^+
E_{zpe}= -297.286508
G= -297.319725

B	0.169503000	-0.483619000	2.380645000
B	0.225736000	2.297838000	0.785224000
B	0.225736000	2.297838000	-0.785224000
B	0.010350000	1.001099000	-1.702014000
B	-0.409729000	-0.458893000	-0.859382000
B	0.178993000	-1.816940000	-1.586825000
B	0.169503000	-0.483619000	-2.380645000
B	0.091349000	-2.057967000	0.000000000
B	0.010350000	1.001099000	1.702014000
B	0.178993000	-1.816940000	1.586825000
B	-0.409729000	-0.458893000	0.859382000
B	-0.441055000	0.978995000	0.000000000

B_{12}^+ (TS)
E_{zpe}= -297.274335

G= -297.307108

B	0.122194000	1.075936000	0.684773000
B	0.939341000	-0.314070000	0.438016000
B	2.487161000	-0.028257000	-0.221888000
B	1.936055000	-1.478632000	-0.188824000
B	-0.872799000	-0.227540000	0.337684000
B	-1.135407000	-1.936540000	-0.091757000
B	0.462004000	-1.984840000	-0.100318000
B	1.591816000	1.293869000	-0.044105000
B	-1.176090000	1.675432000	-0.139780000
B	-2.346511000	0.594215000	-0.194221000
B	-2.317620000	-0.954960000	-0.098152000
B	0.309855000	2.285387000	-0.381428000

B_{12}

E_{zpe}= -297.604246

G= -297.635190

B	-0.776355000	-2.296524000	-0.174721000
B	-2.377026000	0.475918000	-0.174721000
B	-1.600670000	1.820605000	-0.174721000
B	0.000000000	2.015547000	-0.039574000
B	0.841467000	0.485821000	0.389017000
B	2.377026000	0.475918000	-0.174721000
B	1.600670000	1.820605000	-0.174721000
B	1.745515000	-1.007773000	-0.039574000
B	-1.745515000	-1.007773000	-0.039574000
B	0.776355000	-2.296524000	-0.174721000
B	0.000000000	-0.971642000	0.389017000
B	-0.841467000	0.485821000	0.389017000

B_{12} (TS)

E_{zpe}= -297.573127

G= -297.606004

B	0.017743000	0.968144000	0.464811000
B	0.829554000	-0.499348000	0.464671000
B	2.216517000	0.302965000	-0.140158000
B	2.095094000	-1.261359000	-0.184384000
B	-0.847293000	-0.468632000	0.464683000
B	-0.845813000	-2.070950000	-0.140158000
B	0.769328000	-2.100553000	-0.140139000
B	1.434484000	1.716491000	-0.140161000
B	-1.370606000	1.767922000	-0.140136000
B	-2.203904000	0.384008000	-0.140170000
B	-2.139924000	-1.183726000	-0.184385000
B	0.044820000	2.445038000	-0.184474000

B_{13}^-
E_{zpe}= -322.486244
G= -322.519935

B	0.000000000	0.908803000	-0.377899000
B	0.000000000	-0.908803000	-0.377899000
B	0.000000000	0.000000000	1.091180000
B	0.000000000	0.755313000	2.538876000
B	0.000000000	-0.755313000	2.538876000
B	0.000000000	1.770038000	1.262466000
B	0.000000000	-1.770038000	1.262466000
B	0.000000000	2.559112000	-0.081885000
B	0.000000000	-2.559112000	-0.081885000
B	0.000000000	2.111557000	-1.552075000
B	0.000000000	0.758557000	-2.335072000
B	0.000000000	-0.758557000	-2.335072000
B	0.000000000	-2.111557000	-1.552075000

B_{13}^- (TS)
E_{zpe}= -322.484385
G= -322.518706

B	-0.980637000	-0.006345000	-0.008635000
B	0.612361000	-0.847229000	0.020631000
B	0.601075000	0.853663000	0.021414000
B	-2.093129000	1.411774000	0.009517000
B	-0.744887000	2.114294000	-0.011059000
B	-2.674180000	-0.018829000	0.005980000
B	0.827197000	2.476196000	-0.017448000
B	-2.072148000	-1.439830000	0.000653000
B	2.073042000	1.606654000	-0.004486000
B	-0.713667000	-2.124277000	-0.012171000
B	0.863696000	-2.465109000	-0.014862000
B	2.096225000	-1.577082000	0.001320000
B	2.205052000	0.016122000	0.009147000

B_{13}^+
E_{zpe}= -322.128528
G= -322.163213

B	0.896527000	0.435868000	0.000191000
B	-0.896529000	0.435864000	-0.000148000
B	0.000002000	-1.022661000	-0.000047000
B	0.768538000	-2.509605000	-0.000015000
B	-0.768525000	-2.509609000	0.000054000
B	1.789534000	-1.291918000	-0.000107000
B	-1.789527000	-1.291927000	0.000074000
B	2.596074000	0.074006000	-0.000021000

B	-2.596074000	0.073993000	0.000025000
B	2.164452000	1.546127000	0.000034000
B	0.792724000	2.256875000	0.000027000
B	-0.792736000	2.256871000	-0.000032000
B	-2.164460000	1.546116000	-0.000034000

B_{13}^{+} (TS)
E_{zpe}= -322.128344
G= -322.162371

B	-0.982073000	-0.000078000	0.000014000
B	0.558611000	-0.847438000	0.000016000
B	0.558439000	0.847552000	0.000017000
B	-2.078645000	1.413534000	-0.000008000
B	-0.686635000	2.168429000	-0.000006000
B	-2.675086000	-0.000289000	-0.000001000
B	0.846629000	2.494483000	-0.000004000
B	-2.078307000	-1.413972000	-0.000004000
B	2.086478000	1.588074000	-0.000008000
B	-0.686157000	-2.168616000	-0.000004000
B	0.847180000	-2.494305000	-0.000008000
B	2.086827000	-1.587616000	-0.000008000
B	2.202739000	0.000241000	0.000003000

B_{13}
E_{zpe}= -322.395527
G= -322.430509

B	-0.906550000	-0.409372000	0.000007000
B	0.906567000	-0.409335000	0.000001000
B	-0.000022000	1.052939000	0.000022000
B	-0.760495000	2.515405000	-0.000005000
B	0.760391000	2.515437000	-0.000021000
B	-1.777892000	1.273571000	0.000032000
B	1.777839000	1.273644000	-0.000004000
B	-2.576999000	-0.077806000	-0.000019000
B	2.577003000	-0.077700000	-0.000006000
B	-2.142162000	-1.542969000	-0.000014000
B	-0.771631000	-2.285482000	-0.000004000
B	0.771725000	-2.285451000	0.000007000
B	2.142225000	-1.542882000	0.000004000

B_{13} (TS)
E_{zpe}= -322.394950
G= -322.429633

B	0.978605000	-0.000019000	0.000060000
B	-0.584743000	0.848626000	0.000083000
B	-0.584743000	-0.848627000	0.000083000

B	2.078088000	-1.418641000	0.000012000
B	0.707623000	-2.137943000	-0.000032000
B	2.670535000	-0.000033000	0.000001000
B	-0.844528000	-2.477963000	-0.000087000
B	2.078114000	1.418606000	-0.000023000
B	-2.080536000	-1.587574000	-0.000017000
B	0.707688000	2.137935000	-0.000038000
B	-0.844469000	2.477978000	-0.000068000
B	-2.080508000	1.587619000	-0.000009000
B	-2.201126000	0.000035000	0.000035000

B_{14}^-
E_{zpe}= -347.325471
G= -347.361268

B	2.042053000	1.752251000	0.000018000
B	3.200085000	0.763460000	0.000033000
B	3.200060000	-0.763507000	0.000023000
B	2.042066000	-1.752438000	0.000022000
B	0.509569000	-1.584353000	-0.000010000
B	-1.100803000	-1.513111000	-0.000003000
B	-2.699123000	-1.384173000	-0.000013000
B	-3.455784000	-0.000009000	0.000005000
B	-2.699154000	1.384112000	0.000114000
B	-1.100777000	1.512771000	-0.000055000
B	0.509537000	1.584950000	-0.000070000
B	1.564218000	-0.000243000	-0.000036000
B	-0.182834000	0.000382000	0.000005000
B	-1.829116000	-0.000091000	-0.000035000

B_{14}^- (TS)
E_{zpe}= -347.310147
G= -347.345563

B	-0.811779000	-1.545085000	0.000022000
B	-2.384393000	-1.639317000	0.000003000
B	-3.354564000	-0.438414000	-0.000022000
B	-2.948856000	1.052293000	-0.000017000
B	-1.539025000	1.707077000	-0.000003000
B	-0.000001000	1.934058000	0.000021000
B	1.539024000	1.707077000	0.000008000
B	2.948856000	1.052293000	-0.000010000
B	3.354565000	-0.438414000	-0.000023000
B	2.384393000	-1.639317000	-0.000010000
B	0.811779000	-1.545084000	0.000011000
B	-1.691109000	-0.072697000	-0.000014000
B	-0.000001000	-0.061774000	0.000043000
B	1.691110000	-0.072696000	-0.000010000

B_{14}^{+}
E_{zpe}= -346.927272
G= -346.961752

B	0.000002000	0.856139000	0.538060000
B	0.000000000	-0.856141000	0.538058000
B	1.437823000	-0.000004000	0.363657000
B	1.443926000	1.734643000	-0.101802000
B	1.443915000	-1.734645000	-0.101805000
B	-1.437831000	0.000003000	0.363699000
B	0.000000000	2.381051000	-0.184359000
B	2.754314000	0.768811000	-0.256897000
B	-1.443926000	1.734656000	-0.101737000
B	-1.443938000	-1.734653000	-0.101741000
B	-0.000012000	-2.381052000	-0.184364000
B	2.754312000	-0.768821000	-0.256898000
B	-2.754295000	-0.768806000	-0.256938000
B	-2.754292000	0.768817000	-0.256935000

B_{14}^{+} (TS)
E_{zpe}= -346.911770
G= -346.947058

B	0.012069000	-0.805019000	0.884289000
B	-0.012068000	0.805022000	0.884287000
B	-1.382397000	-0.027531000	0.334511000
B	-0.829747000	-1.862013000	-0.157724000
B	-2.258256000	1.427351000	-0.297216000
B	1.382400000	0.027529000	0.334514000
B	0.754279000	-1.921475000	-0.165406000
B	-2.340422000	-1.376730000	-0.314188000
B	2.258255000	-1.427353000	-0.297218000
B	0.829746000	1.862016000	-0.157725000
B	-0.754280000	1.921473000	-0.165408000
B	-2.964001000	0.041435000	-0.284263000
B	2.340421000	1.376729000	-0.314187000
B	2.964000000	-0.041436000	-0.284265000

B_{15}^{-}
E_{zpe}= -372.140388
G= -372.176592

B	0.127346000	0.855108000	0.097349000
B	0.097553000	-0.843514000	0.080164000
B	-1.506520000	-0.057741000	-0.196996000
B	-1.043024000	2.128909000	0.014019000
B	-1.217225000	-1.956504000	0.052388000
B	1.622599000	-0.038840000	0.307533000

B	0.459201000	2.472474000	-0.030172000
B	-3.189128000	0.097366000	-0.097187000
B	1.828310000	1.684990000	0.023812000
B	1.669605000	-1.779530000	-0.039132000
B	0.255560000	-2.480912000	-0.057148000
B	-2.654572000	-1.319998000	0.111617000
B	2.965394000	-0.862867000	-0.150379000
B	3.039889000	0.673501000	-0.097548000
B	-2.454987000	1.427557000	-0.018321000

B_{15}^- (TS)
E_{zpe}= -372.139041
G= -372.174039

B	-0.000059000	0.852635000	-0.000065000
B	-0.000028000	-0.855087000	-0.000037000
B	-1.558059000	-0.095034000	-0.256165000
B	-2.122815000	1.570160000	-0.064601000
B	-0.000063000	-2.510854000	-0.000003000
B	1.558015000	-0.095047000	0.256153000
B	-0.758775000	2.378220000	0.000159000
B	-2.825610000	-1.107795000	0.164874000
B	0.758929000	2.378107000	-0.000209000
B	2.825536000	-1.107915000	-0.164848000
B	1.443565000	-1.880313000	-0.062551000
B	-1.443679000	-1.880273000	0.062533000
B	3.122129000	0.391473000	0.006451000
B	2.123001000	1.570098000	0.064644000
B	-3.122086000	0.391626000	-0.006335000

B_{15}^+
E_{zpe}= -371.750211
G= -371.786783

B	0.101438000	0.827382000	0.000628000
B	0.101055000	-0.829081000	0.001594000
B	-1.469045000	0.003270000	0.002361000
B	-1.122463000	1.998456000	0.000693000
B	-1.122762000	-2.002571000	0.000646000
B	1.594311000	0.000865000	0.010049000
B	0.358703000	2.472389000	-0.000599000
B	-3.221295000	0.000333000	-0.002100000
B	1.782562000	1.777916000	-0.000318000
B	1.780867000	-1.776615000	-0.000709000
B	0.358592000	-2.473749000	-0.000132000
B	-2.606160000	-1.383664000	-0.001866000
B	3.035887000	-0.760336000	-0.004938000
B	3.036663000	0.760358000	-0.003485000

B -2.608353000 1.385047000 -0.001826000

B_{15}^{+} (TS)
E_{zpe}= -371.747932
G= -371.783538
B 0.000059000 0.804209000 0.000842000
B 0.000009000 -0.851997000 0.000730000
B 1.529707000 -0.069627000 0.000363000
B 2.214091000 1.638658000 -0.000611000
B 0.000020000 -2.514363000 -0.000184000
B -1.529718000 -0.069634000 -0.000064000
B 0.764805000 2.321905000 -0.000206000
B 2.851755000 -1.101718000 0.000449000
B -0.764848000 2.321819000 0.000081000
B -2.851735000 -1.101760000 -0.000679000
B -1.440329000 -1.890243000 -0.000627000
B 1.440382000 -1.890272000 0.000397000
B -3.139168000 0.382149000 0.000153000
B -2.214180000 1.638655000 0.000237000
B 3.139149000 0.382220000 -0.000882000

B_{15}
E_{zpe}= -372.023001
G= -372.059835
B 0.114140000 0.836245000 0.096430000
B 0.113751000 -0.835626000 0.096158000
B -1.479511000 -0.002064000 -0.081630000
B -1.128359000 2.002708000 0.011888000
B -1.129990000 -1.999051000 0.011814000
B 1.608891000 -0.000455000 0.194940000
B 0.356572000 2.466717000 -0.054465000
B -3.203863000 0.000993000 -0.077246000
B 1.764056000 1.752739000 -0.021901000
B 1.762753000 -1.754147000 -0.022143000
B 0.354505000 -2.466492000 -0.054108000
B -2.589265000 -1.383216000 0.023231000
B 3.020913000 -0.765140000 -0.073036000
B 3.021617000 0.762916000 -0.072962000
B -2.586210000 1.383871000 0.023030000

B_{15} (TS)
E_{zpe}= -372.020740
G= -372.056682
B 0.000001000 0.831967000 -0.000102000
B 0.000030000 -0.852576000 -0.000177000
B -1.541401000 -0.085162000 -0.142026000

B	-2.162557000	1.602273000	0.001138000
B	0.000030000	-2.509533000	-0.000032000
B	1.541401000	-0.085146000	0.142068000
B	-0.760186000	2.355421000	0.026644000
B	-2.842396000	-1.110619000	0.063154000
B	0.760120000	2.355438000	-0.026675000
B	2.842440000	-1.110563000	-0.063016000
B	1.442852000	-1.881620000	-0.016134000
B	-1.442808000	-1.881621000	0.016150000
B	3.125252000	0.384752000	0.002072000
B	2.162493000	1.602310000	-0.001089000
B	-3.125271000	0.384680000	-0.001976000

B_{16}^-
E_{zpe}= -396.962021
G= -396.999040

B	-0.767054000	-0.000001000	0.021216000
B	-0.000049000	1.557813000	0.001525000
B	1.635617000	1.608803000	-0.042511000
B	3.206997000	1.405560000	0.055528000
B	3.955697000	-0.000001000	0.074648000
B	3.206996000	-1.405560000	0.055523000
B	1.635617000	-1.608804000	-0.042515000
B	-0.000048000	-1.557812000	0.001527000
B	-1.635650000	-1.609001000	0.043321000
B	-3.206537000	-1.405349000	-0.059430000
B	-3.955123000	0.000000000	-0.081193000
B	-3.206537000	1.405347000	-0.059431000
B	-1.635651000	1.609002000	0.043317000
B	-2.374503000	0.000001000	0.221746000
B	0.766697000	0.000002000	-0.014675000
B	2.373530000	-0.000001000	-0.218596000

B_{16}^- (TS)
E_{zpe}= -396.897175
G= -396.934163

B	1.124378000	0.147313000	0.247245000
B	0.400873000	-1.396318000	-0.112710000
B	-1.188858000	-1.571811000	-0.025372000
B	-2.754683000	-1.764089000	0.002558000
B	-3.803346000	-0.629185000	-0.018127000
B	-3.508286000	0.900869000	-0.018703000
B	-2.147460000	1.641208000	-0.033699000
B	-0.633216000	1.987165000	-0.103100000
B	0.919968000	1.897458000	-0.039821000
B	2.401890000	1.357835000	0.076825000

B	3.659250000	0.429341000	-0.424682000
B	3.538663000	-1.150960000	-0.282126000
B	2.017808000	-1.556388000	0.002820000
B	2.664021000	-0.175817000	0.718584000
B	-0.493975000	0.037374000	-0.012349000
B	-2.197026000	-0.153996000	0.022658000

B_{16}
E_{zpe}= -396.844258
G= -396.880199

B	0.786199000	0.000009000	0.014021000
B	-0.000031000	1.573559000	0.000590000
B	-1.614885000	1.578632000	0.071792000
B	-3.182206000	1.374854000	-0.119225000
B	-3.951399000	-0.000007000	-0.093535000
B	-3.182191000	-1.374862000	-0.119224000
B	-1.614873000	-1.578619000	0.071820000
B	-0.000012000	-1.573538000	0.000619000
B	1.614840000	-1.578507000	-0.071119000
B	3.182540000	-1.374982000	0.117611000
B	3.951619000	0.000003000	0.091145000
B	3.182536000	1.374994000	0.117633000
B	1.614823000	1.578488000	-0.071084000
B	2.367469000	0.000012000	-0.378850000
B	-0.786395000	-0.000047000	-0.011893000
B	-2.368035000	0.000011000	0.379698000

B_{16} (TS)
E_{zpe}= -396.786872
G= -396.823321

B	1.100431000	0.080297000	0.265588000
B	0.354334000	-1.477637000	0.010710000
B	-1.249211000	-1.587572000	-0.018928000
B	-2.817677000	-1.708676000	-0.051054000
B	-3.825156000	-0.527837000	-0.105299000
B	-3.460099000	0.972288000	0.006357000
B	-2.065118000	1.657993000	0.034258000
B	-0.548657000	1.995554000	0.033754000
B	0.994694000	1.893275000	-0.084838000
B	2.473584000	1.356292000	-0.058720000
B	3.687809000	0.384944000	-0.464059000
B	3.427366000	-1.157196000	-0.354770000
B	1.958854000	-1.574755000	0.132472000
B	2.662783000	-0.147267000	0.712546000
B	-0.512011000	-0.036960000	0.070906000

B -2.181925000 -0.122743000 -0.128923000

B_{17}^-
E_{zpe}= -421.805577
G= -421.842910
B -0.681985000 1.689290000 0.000000000
B -0.905781000 3.318217000 0.000000000
B -0.572502000 0.000000000 0.000000000
B -0.681986000 -1.689290000 0.000000000
B -0.905781000 -3.318217000 0.000000000
B -2.147229000 2.413731000 0.000000000
B -2.145844000 0.810287000 0.000000000
B -2.145846000 -0.810288000 0.000000000
B -2.147229000 -2.413731000 0.000000000
B 0.615604000 2.896200000 0.000000000
B 0.903046000 0.944007000 0.000000000
B 0.903046000 -0.944007000 0.000000000
B 0.615604000 -2.896199000 0.000000000
B 2.030382000 2.204504000 0.000000000
B 2.618060000 0.814736000 0.000000000
B 2.618060000 -0.814735000 0.000000000
B 2.030382000 -2.204504000 0.000000000}

B_{17}^- (TS)
E_{zpe}= -421.783321
G= -421.819909
B 0.286880000 -0.736378000 0.552230000
B 1.347554000 -1.969798000 -0.061663000
B -0.212179000 -2.261779000 0.072943000
B 1.818408000 -0.154748000 -0.037577000
B -1.363451000 -0.908826000 -0.056765000
B 0.507249000 0.871289000 0.564954000
B -1.217638000 0.930632000 -0.002529000
B -0.019504000 2.338766000 -0.025127000
B -1.592327000 2.587791000 0.077228000
B 2.845169000 -1.523283000 -0.118966000
B -1.788295000 -2.533792000 0.028462000
B 3.493209000 -0.134856000 -0.174187000
B -2.902904000 -1.519073000 -0.196837000
B 2.868434000 1.272045000 -0.153153000
B -2.848518000 0.056690000 -0.227236000
B 1.523427000 2.056821000 -0.159623000
B -2.745516000 1.628501000 -0.082155000

B_{17}
E_{zpe}= -421.662290

G= -421.700623

B	2.026708000	2.183252000	0.000080000
B	0.444715000	2.434676000	0.000119000
B	-1.140120000	2.629922000	-0.000240000
B	-2.338746000	1.707616000	-0.000193000
B	-3.193639000	0.389849000	0.000046000
B	-3.270347000	-1.132607000	0.000024000
B	-2.215600000	-2.229175000	-0.000047000
B	-0.639005000	-2.090390000	0.000177000
B	0.983703000	-2.101127000	-0.000188000
B	2.584159000	-2.003796000	-0.000441000
B	3.409419000	-0.692746000	-0.000039000
B	2.810354000	0.806839000	0.000368000
B	1.033230000	0.878824000	-0.000175000
B	-0.714988000	1.011304000	-0.000243000
B	-1.637090000	-0.625767000	0.000170000
B	0.070477000	-0.562489000	0.000604000
B	1.786769000	-0.604185000	-0.000021000

B_{17} (TS)

E_{zpe}= -421.638611

G= -421.676247

B	0.350981000	-0.804769000	0.669759000
B	1.408731000	-1.932659000	-0.099444000
B	-0.120255000	-2.296610000	0.104699000
B	1.811934000	0.000072000	0.047852000
B	-1.263748000	-0.897162000	-0.074429000
B	0.351257000	0.805089000	0.669755000
B	-1.263588000	0.897189000	-0.073682000
B	-0.119758000	2.296886000	0.104203000
B	-1.676697000	2.569280000	0.047760000
B	2.872167000	-1.386082000	-0.228918000
B	-1.677153000	-2.569178000	0.047252000
B	3.510543000	-0.000292000	-0.230387000
B	-2.819672000	-1.574769000	-0.190970000
B	2.872516000	1.385682000	-0.229422000
B	-2.826853000	0.000163000	-0.273548000
B	1.409003000	1.932131000	-0.100546000
B	-2.819408000	1.575028000	-0.189934000

B_{18}^-

E_{zpe}= -446.628141

G= -446.665691

B	0.502775000	0.392806000	0.870821000
B	0.502775000	0.392806000	-0.870821000
B	-1.005410000	0.391781000	0.000000000

B	-0.915719000	-0.095260000	-1.586111000
B	1.831389000	-0.095335000	0.000000000
B	-0.915719000	-0.095260000	1.586111000
B	-2.479685000	-0.018560000	0.821914000
B	-2.479685000	-0.018560000	-0.821914000
B	0.528080000	-0.017728000	-2.558512000
B	1.951544000	-0.018804000	-1.736513000
B	1.951544000	-0.018804000	1.736513000
B	0.528080000	-0.017728000	2.558512000
B	-0.948193000	-0.129953000	3.208121000
B	-2.304151000	-0.130372000	2.425254000
B	-2.304151000	-0.130372000	-2.425254000
B	-0.948193000	-0.129953000	-3.208121000
B	3.252361000	-0.130352000	-0.782841000
B	3.252361000	-0.130352000	0.782841000

B_{18}^- (TS)
E_{zpe}= -446.562305
G= -446.600152

B	0.000049000	-0.882714000	0.014108000
B	-0.837613000	0.662231000	0.130333000
B	0.837168000	0.662439000	0.130012000
B	-0.000336000	1.947306000	0.673457000
B	-1.811050000	-0.618948000	0.310259000
B	1.811121000	-0.618427000	0.310186000
B	3.364440000	-0.223085000	-0.189640000
B	2.506207000	1.121694000	-0.096974000
B	-1.411742000	2.321693000	-0.095586000
B	-2.506777000	1.120824000	-0.096751000
B	-1.515310000	-2.339596000	-0.030533000
B	0.000668000	-2.658077000	-0.118580000
B	1.516568000	-2.339330000	-0.030358000
B	2.952293000	-1.703448000	-0.102874000
B	1.410846000	2.322153000	-0.095866000
B	-0.000601000	3.154139000	-0.418302000
B	-3.364436000	-0.224358000	-0.189738000
B	-2.951495000	-1.704496000	-0.103154000

B_{18}
E_{zpe}= -446.496852
G= -446.533833

B	0.510299000	0.348675000	0.883880000
B	0.510299000	0.348675000	-0.883880000
B	-1.020663000	0.347847000	0.000000000
B	-0.902844000	-0.205445000	-1.563800000
B	1.805679000	-0.205301000	0.000000000

B	-0.902844000	-0.205445000	1.563800000
B	-2.466550000	-0.007872000	0.834230000
B	-2.466550000	-0.007872000	-0.834230000
B	0.510914000	-0.007107000	-2.553206000
B	1.955676000	-0.007547000	-1.718994000
B	1.955676000	-0.007547000	1.718994000
B	0.510914000	-0.007107000	2.553206000
B	-0.942597000	-0.063821000	3.206284000
B	-2.305428000	-0.063826000	2.419489000
B	-2.305428000	-0.063826000	-2.419489000
B	-0.942597000	-0.063821000	-3.206284000
B	3.248022000	-0.064331000	-0.786809000
B	3.248022000	-0.064331000	0.786809000

B_{18} (TS)
E_{zpe}= -446.440736
G= -446.477775

B	0.000072000	-0.910853000	-0.018130000
B	-0.860066000	0.678392000	0.221444000
B	0.859945000	0.678399000	0.221092000
B	0.000009000	1.931538000	0.741652000
B	-1.862987000	-0.592476000	0.342207000
B	1.863080000	-0.592272000	0.342231000
B	3.402243000	-0.209745000	-0.232653000
B	2.537088000	1.115148000	-0.063679000
B	-1.413574000	2.286403000	-0.108937000
B	-2.537212000	1.115023000	-0.063399000
B	-1.499206000	-2.270994000	-0.025512000
B	0.000085000	-2.657345000	-0.021903000
B	1.499349000	-2.270863000	-0.025098000
B	2.947232000	-1.674467000	-0.204441000
B	1.413388000	2.286449000	-0.109302000
B	-0.000150000	2.972192000	-0.558207000
B	-3.402207000	-0.209921000	-0.232612000
B	-2.947090000	-1.674611000	-0.204753000

B_{19}^-
E_{zpe}= -471.443229
G= -471.483725

B	0.000000000	0.000000000	-0.001723000
B	0.000000000	0.953634000	-1.315761000
B	0.000000000	-0.953634000	-1.315761000
B	0.000000000	1.566988000	0.488878000
B	0.000000000	-1.566988000	0.488878000
B	0.000000000	0.000000000	1.606935000
B	0.000000000	0.000000000	3.266409000

B	0.000000000	1.434370000	2.748156000
B	0.000000000	-1.434370000	2.748156000
B	0.000000000	0.789022000	-3.092993000
B	0.000000000	-0.789022000	-3.092993000
B	0.000000000	-2.159077000	-2.465766000
B	0.000000000	-2.698836000	1.819819000
B	0.000000000	2.159077000	-2.465766000
B	0.000000000	2.698836000	1.819819000
B	0.000000000	3.261925000	0.434818000
B	0.000001000	2.797047000	-1.052962000
B	0.000000000	-3.261925000	0.434818000
B	-0.000001000	-2.797047000	-1.052962000

B_{19}^- (TS)
E_{zpe}= -471.443291
G= -471.482601

B	0.001025000	0.000000000	0.000000000
B	1.331460000	-0.949674000	0.000000000
B	1.331461000	0.949672000	0.000000000
B	-0.488977000	1.537147000	0.000000000
B	-1.645262000	0.000001000	0.000000000
B	-0.488978000	-1.537147000	0.000000000
B	2.973950000	0.000000000	0.000000000
B	0.361373000	-3.132303000	0.000000000
B	-2.273246000	-2.006053000	0.000000000
B	-2.273246000	2.006052000	0.000000000
B	1.856600000	2.636545000	0.000000000
B	-3.196622000	0.746368000	0.000000000
B	-1.151535000	-3.059548000	0.000000000
B	1.856600000	-2.636545000	0.000000000
B	2.896090000	1.554325000	0.000000000
B	-1.151535000	3.059549000	0.000000000
B	-3.196622000	-0.746368000	0.000000000
B	0.361374000	3.132305000	0.000000000
B	2.896090000	-1.554325000	0.000000000

B_{19}
E_{zpe}= -471.303340
G= -471.342820

B	3.722272000	-0.001505000	0.085328000
B	3.106465000	1.379233000	0.000484000
B	1.675547000	1.968346000	-0.026153000
B	0.226917000	2.609256000	-0.034049000
B	-1.249537000	3.226318000	-0.048966000
B	-2.572756000	2.411680000	-0.008142000
B	-2.671522000	0.820239000	0.002796000

B	-2.672031000	-0.817875000	0.002741000
B	-2.575035000	-2.409391000	-0.008613000
B	-1.252597000	-3.225204000	-0.049517000
B	0.224499000	-2.609589000	-0.034197000
B	1.673910000	-1.971494000	-0.025611000
B	3.104170000	-1.381145000	0.001170000
B	-1.149146000	-1.609758000	0.210996000
B	-1.131769000	0.000375000	-0.071615000
B	-1.147613000	1.610706000	0.210150000
B	0.369992000	-0.854535000	-0.137215000
B	0.370504000	0.853911000	-0.137390000
B	1.947732000	0.000432000	0.067803000

B_{19} (TS)
E_{zpe}= -471.294482
G= -471.333926

B	-0.779865000	3.386795000	0.083204000
B	0.779853000	3.386795000	0.083243000
B	1.701322000	2.104462000	0.043436000
B	2.590693000	0.775355000	-0.067481000
B	3.444326000	-0.540671000	-0.112302000
B	2.951739000	-1.984262000	-0.076729000
B	1.518343000	-2.564594000	0.053807000
B	0.000007000	-2.784764000	0.237575000
B	-1.518335000	-2.564596000	0.053866000
B	-2.951736000	-1.984269000	-0.076666000
B	-3.444326000	-0.540680000	-0.112301000
B	-2.590695000	0.775346000	-0.067520000
B	-1.701327000	2.104461000	0.043372000
B	-1.776056000	-0.808857000	-0.201317000
B	0.000001000	-0.987421000	0.233339000
B	1.776056000	-0.808847000	-0.201319000
B	-0.869620000	0.548267000	0.139297000
B	0.869620000	0.548267000	0.139347000
B	0.000000000	1.939212000	-0.194851000

B_{20}^-
E_{zpe}= -496.235376
G= -496.277048

B	-0.910870000	-3.274057000	0.000036000
B	0.670896000	-2.969256000	0.000087000
B	2.221217000	-2.581778000	-0.000039000
B	-2.116359000	-2.205389000	-0.000132000
B	-0.462445000	-1.666962000	0.000024000
B	1.145196000	-1.313990000	0.000015000
B	2.866089000	-1.128250000	-0.000041000

B	-3.245116000	-1.075809000	0.000021000
B	-1.673761000	-0.532916000	0.000048000
B	-0.005600000	-0.022745000	-0.000103000
B	1.698253000	0.322637000	0.000026000
B	3.381762000	0.375029000	0.000000000
B	-3.068166000	0.495148000	0.000049000
B	-2.693505000	2.039602000	-0.000017000
B	-1.428609000	2.902557000	-0.000018000
B	0.120102000	3.278741000	0.000001000
B	1.586138000	2.883281000	0.000021000
B	2.713960000	1.757505000	0.000021000
B	-1.251140000	1.150792000	0.000008000
B	0.451960000	1.565859000	-0.000008000

B_{20}^- (TS)
E_{zpe}= -496.235285
G= -496.275387

B	-1.604457000	-2.997377000	0.000007000
B	0.000087000	-3.039566000	0.000004000
B	1.604638000	-2.997285000	0.000024000
B	-2.548116000	-1.700047000	0.000004000
B	-0.819353000	-1.528416000	-0.000101000
B	0.819434000	-1.528376000	0.000054000
B	2.548226000	-1.699883000	0.000027000
B	-3.402489000	-0.355075000	0.000032000
B	-1.749984000	-0.114914000	-0.000054000
B	0.000009000	-0.020523000	-0.000073000
B	1.750008000	-0.114896000	-0.000030000
B	3.402524000	-0.354854000	0.000049000
B	-2.961446000	1.138395000	0.000057000
B	-2.179464000	2.523747000	0.000052000
B	-0.797334000	3.159818000	0.000017000
B	0.797059000	3.159817000	-0.000020000
B	2.179318000	2.523977000	-0.000010000
B	2.961243000	1.138588000	0.000026000
B	-0.877759000	1.403430000	-0.000001000
B	0.877857000	1.403439000	-0.000064000

B_{21}^-
E_{zpe}= -521.049032
G= -521.090357

B	0.965617000	0.000001000	0.190107000
B	4.043073000	0.787026000	-0.100532000
B	-2.935692000	2.197412000	-0.083772000
B	-3.553175000	-0.809609000	-0.075993000
B	-0.065788000	1.538935000	0.079743000

B	4.043072000	-0.787040000	-0.100518000
B	1.412438000	-2.553489000	-0.037572000
B	2.835132000	1.756203000	-0.039807000
B	-0.065793000	-1.538932000	0.079742000
B	1.412448000	2.553487000	-0.037529000
B	0.053436000	-3.217181000	-0.070148000
B	-1.447794000	-2.748923000	-0.059835000
B	-2.935702000	-2.197406000	-0.083747000
B	-0.560889000	0.000001000	0.313963000
B	2.835124000	-1.756208000	-0.039801000
B	0.053447000	3.217181000	-0.070157000
B	-1.447782000	2.748923000	-0.059846000
B	-3.553173000	0.809618000	-0.075989000
B	2.591083000	-0.000003000	0.101535000
B	-1.839541000	0.996145000	0.085086000
B	-1.839542000	-0.996140000	0.085070000

B_{21}^- (TS)

E_{zpe}= -521.014819

G= -521.055805

B	-0.873164000	-0.000032000	0.225599000
B	-3.547062000	-1.400282000	-0.096554000
B	3.364780000	-1.591263000	-0.185698000
B	3.365852000	1.589593000	-0.185196000
B	0.149920000	-1.470699000	0.185392000
B	-4.176925000	0.001139000	-0.121475000
B	-2.252969000	2.276920000	-0.070591000
B	-2.254724000	-2.275490000	-0.070010000
B	0.150058000	1.470530000	0.185852000
B	-0.791861000	-2.861651000	-0.062301000
B	-0.789893000	2.861937000	-0.062757000
B	0.698711000	3.139839000	-0.121288000
B	2.201132000	2.593728000	-0.156697000
B	0.631282000	-0.000113000	0.587924000
B	-3.545509000	1.401786000	-0.096940000
B	0.696605000	-3.139959000	-0.121365000
B	2.199267000	-2.594577000	-0.157146000
B	3.447095000	-0.000868000	-0.130554000
B	-2.524142000	0.000074000	0.034861000
B	1.925569000	-0.925958000	0.209281000
B	1.925980000	0.925344000	0.209662000