

## Supplementary Information

### **Pivotal role of B<sub>12</sub>-core in the structural evolution of B<sub>52</sub>-B<sub>64</sub> clusters**

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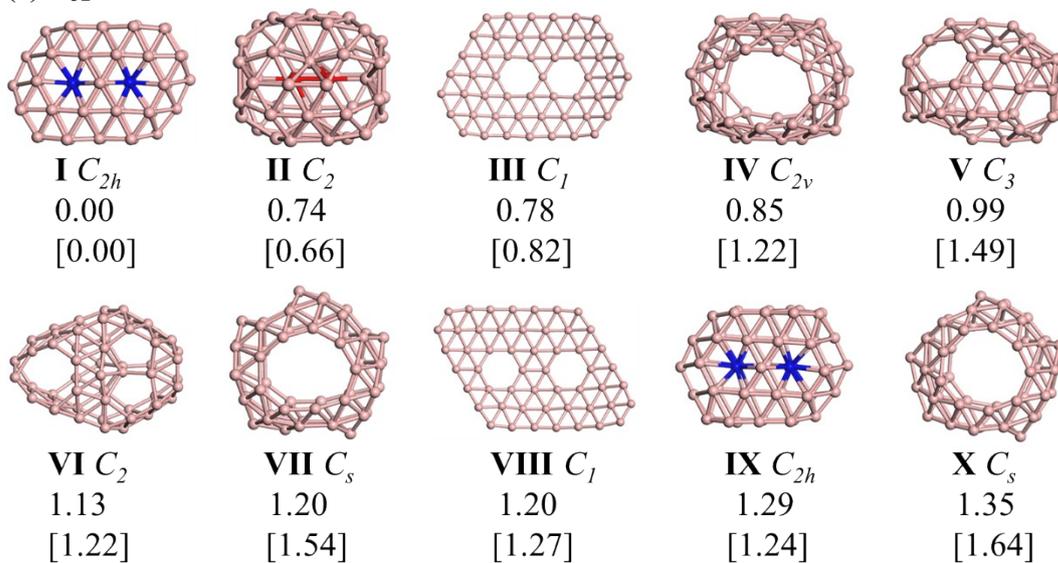
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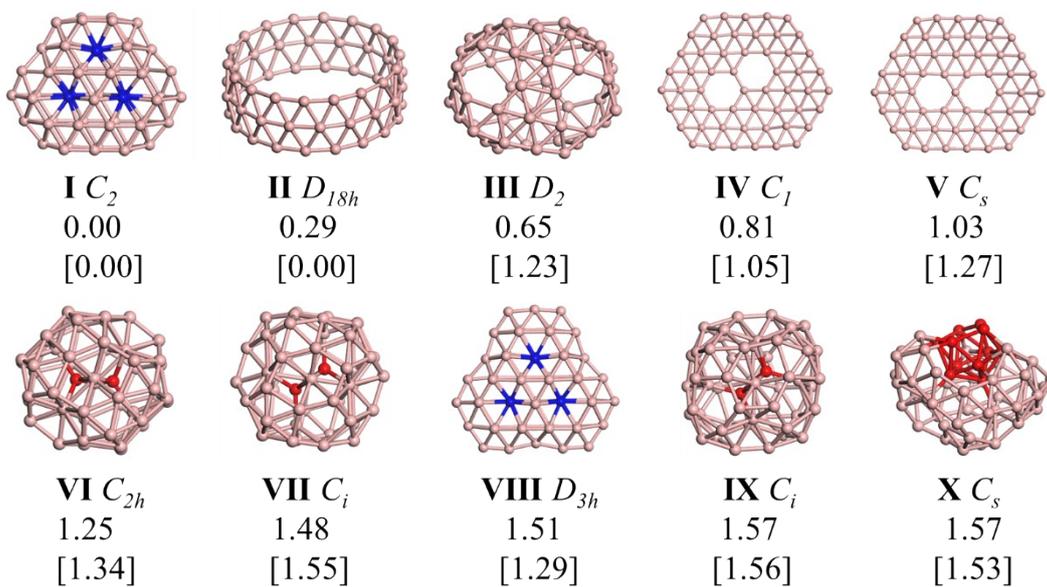
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**Fig. S1** The low-energy isomers of (a) B<sub>52</sub>, (b) B<sub>54</sub>, (c) B<sub>56</sub>, (d) B<sub>58</sub>, (e) B<sub>60</sub>, (f) B<sub>62</sub>, and (g) B<sub>64</sub> clusters obtained from HSE06/6-311+G\* and TPSSh/6-311+G\* (in square brackets) calculations, along with the cluster symmetry and relative energy (in eV). The inner atoms of core-shell structures are highlighted in red, and the out-of-plane atoms of bilayer structures are highlighted in blue.

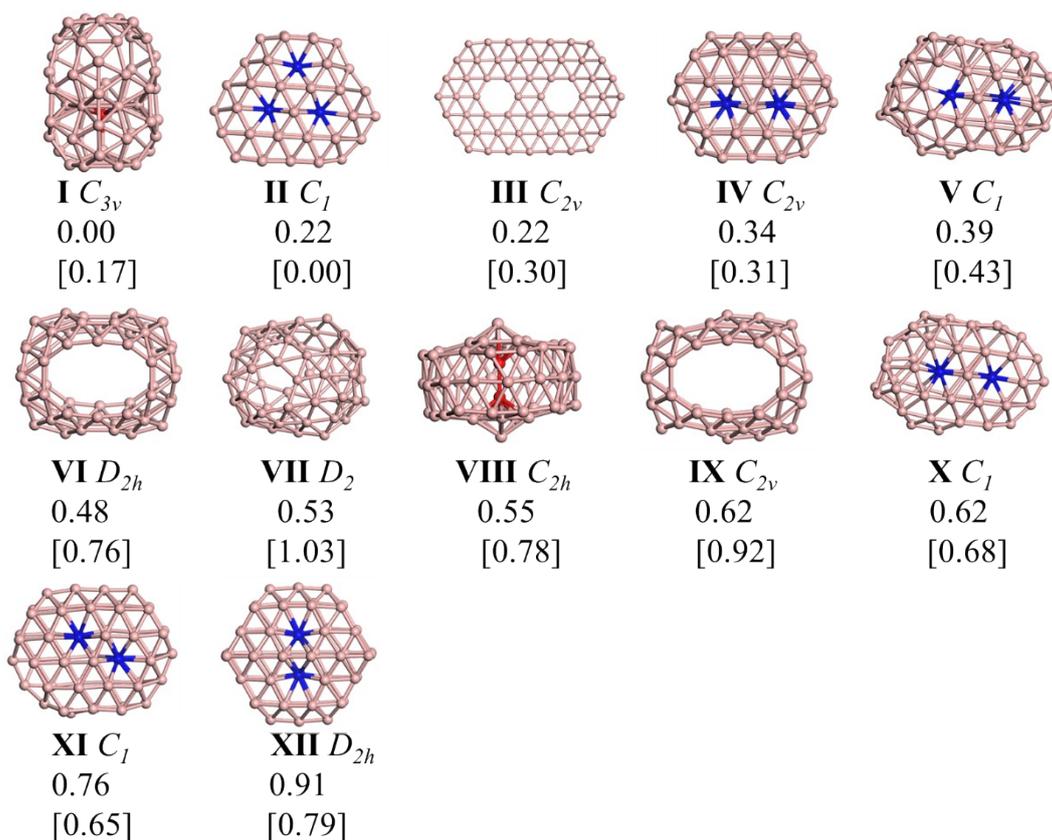
(a) B<sub>52</sub>



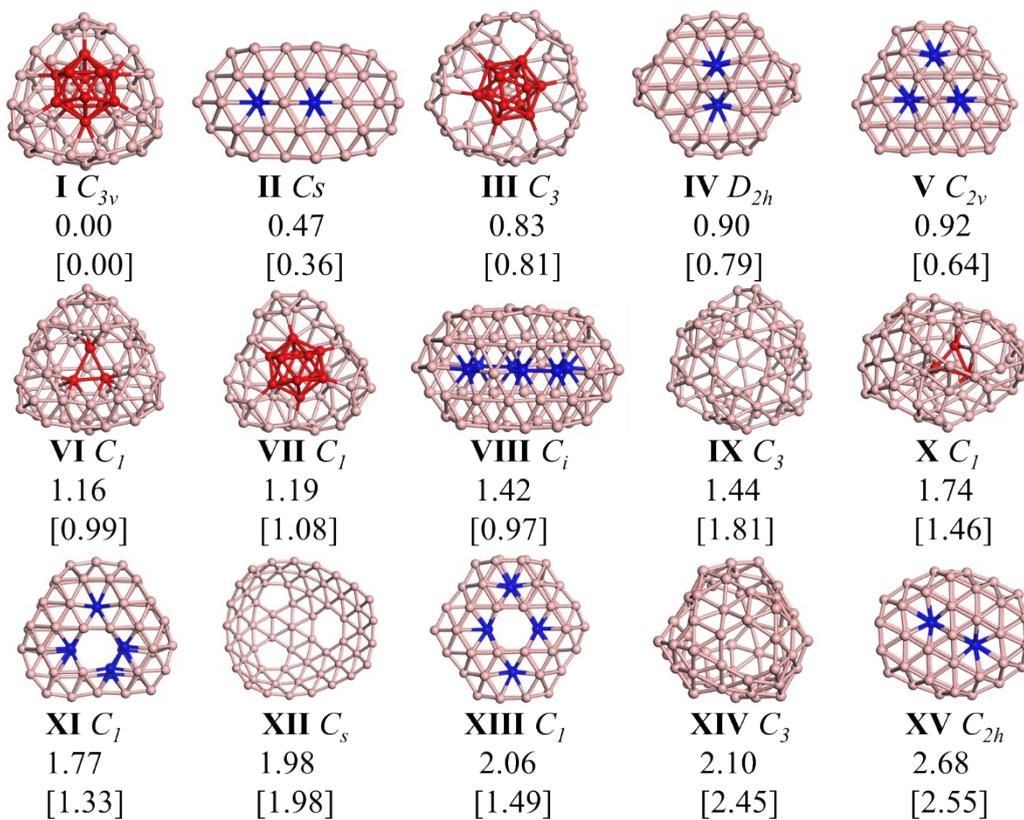
(b) B<sub>54</sub>



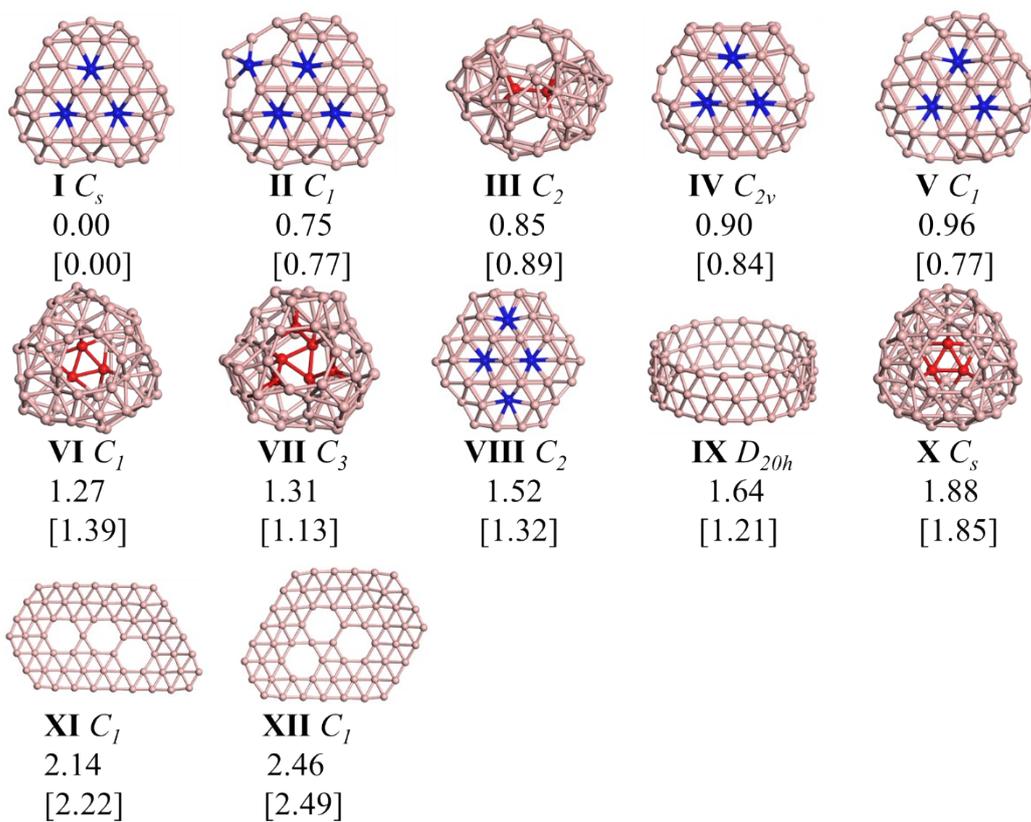
(c) B<sub>56</sub>



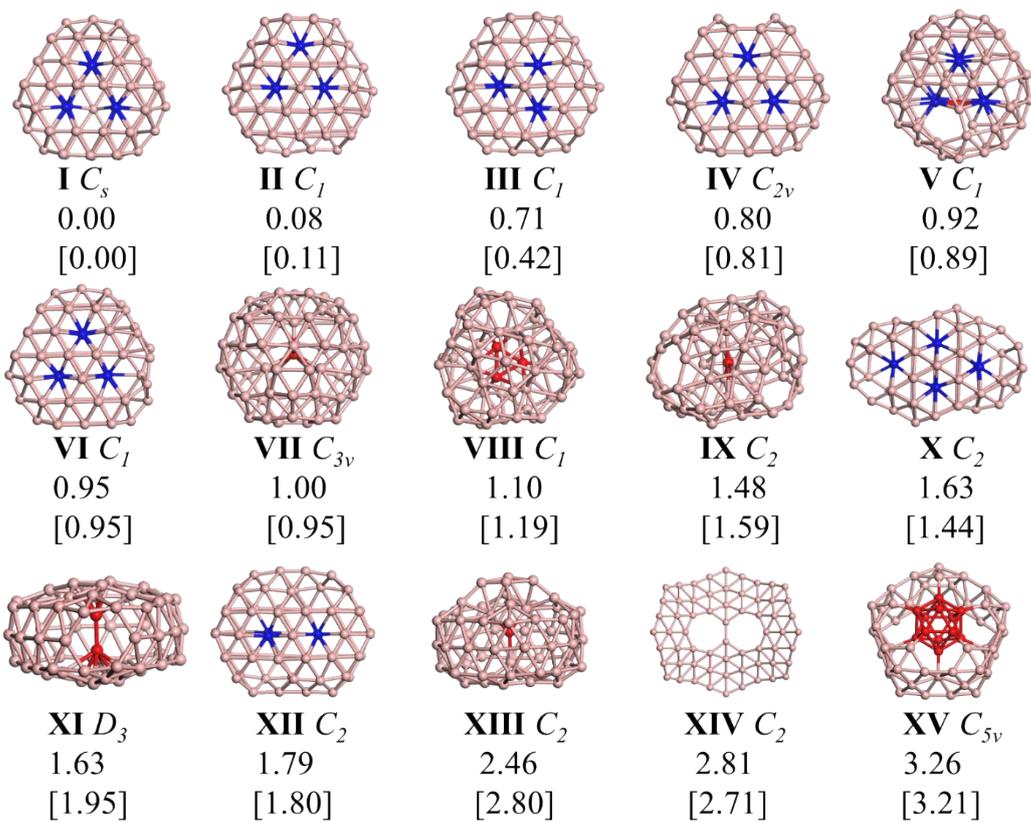
(d) B<sub>58</sub>



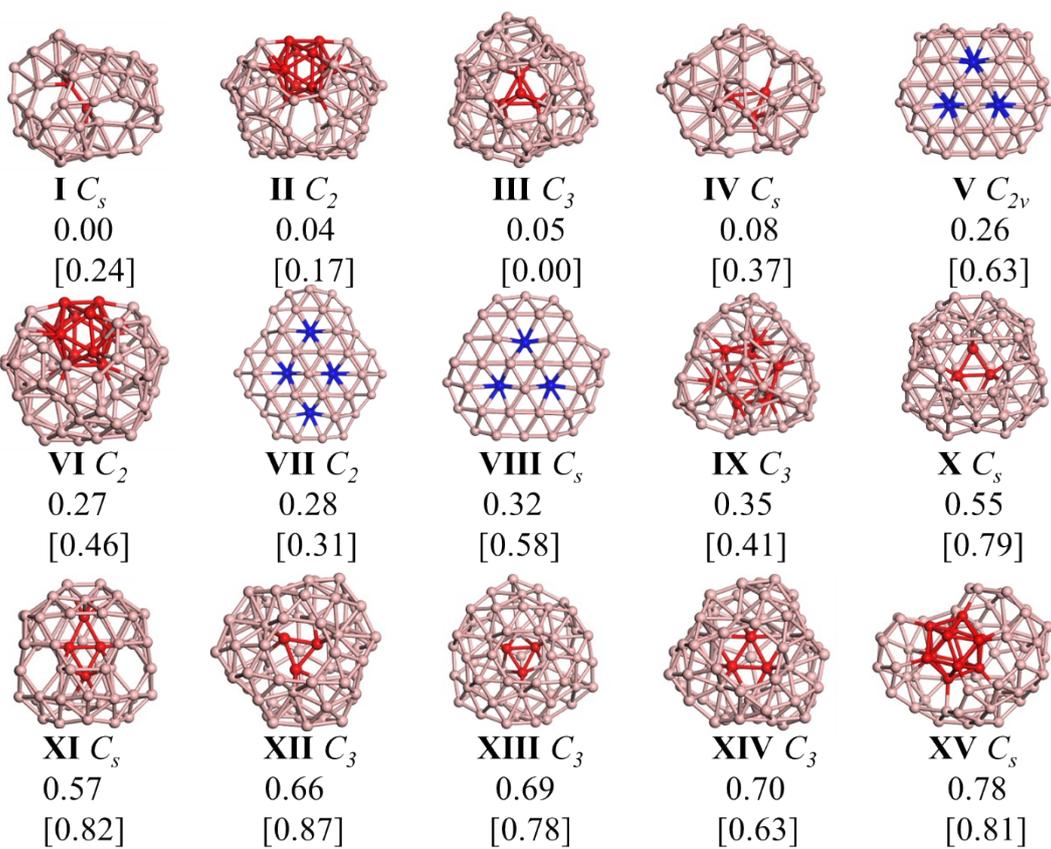
(e) B<sub>60</sub>

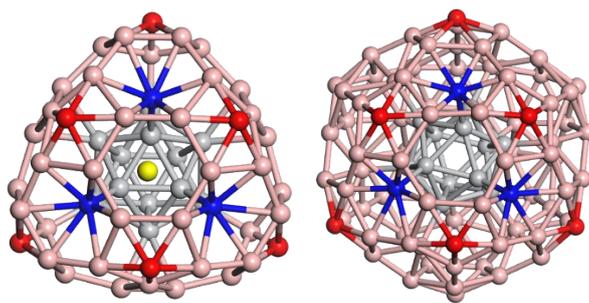


(f) B<sub>62</sub>



(g) B<sub>64</sub>

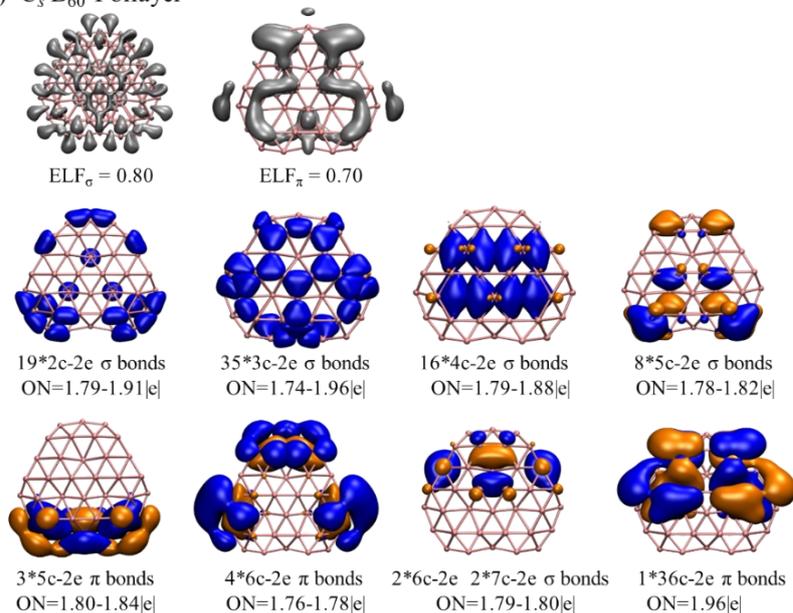




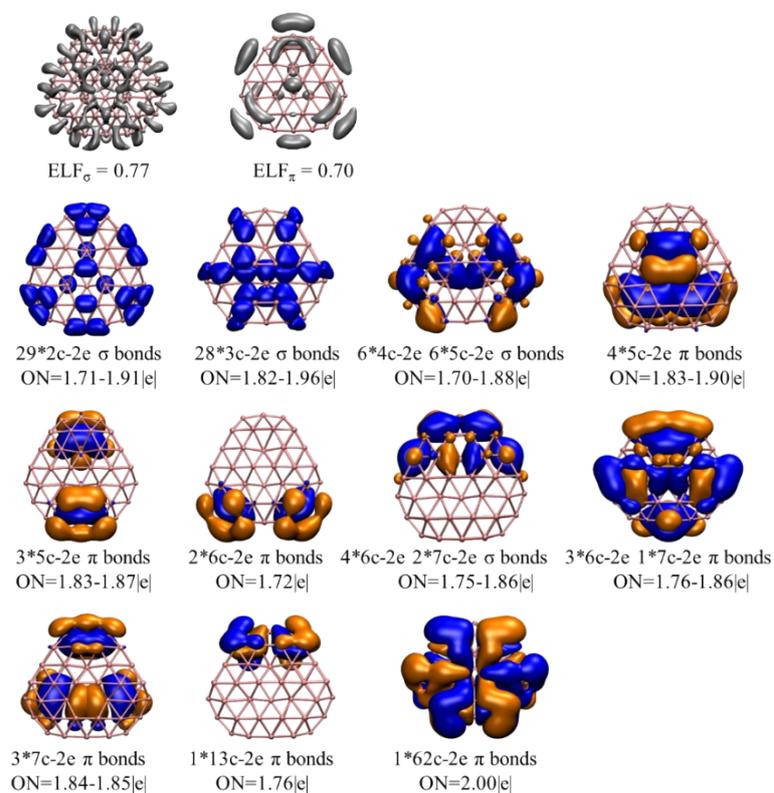
**Fig. S2** Structural comparison between core-shell  $B_{58}$  and  $B_{96}$  clusters. Atoms highlighted in red, blue (yellow), and gray are pentagon capped B, hexagon capped B and core B, respectively.

**Fig. S3** ELF and AdNDP chemical bonding analyses of (a)  $C_s$  B<sub>60</sub>-I bilayer, (b)  $C_s$  B<sub>62</sub>-I bilayer, and (c) core-shell  $C_2$  B<sub>64</sub>-II clusters with a closed electronic shell. ON denotes the occupation number.

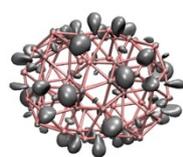
(a)  $C_s$  B<sub>60</sub>-I bilayer



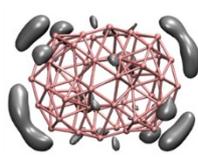
(b)  $C_s$  B<sub>62</sub>-I bilayer



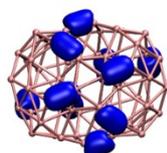
(c)  $C_2$  core-shell  $B_{64}$ -II



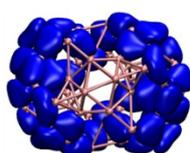
$ELF_{\sigma} = 0.85$



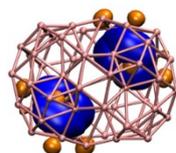
$ELF_{\pi} = 0.70$



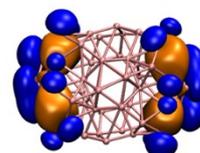
12\*2c-2e  $\sigma$  bonds  
ON=1.88-1.95|e|



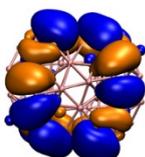
48\*3c-2e  $\sigma$  bonds  
ON=1.73-1.98|e|



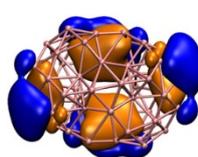
6\*4c-2e  $\sigma$  bonds  
ON=1.56-1.82|e|



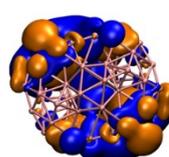
4\*5c-2e  $\sigma$  bonds  
ON=1.78-1.81|e|



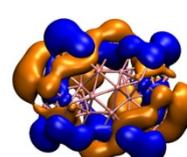
6\*5c-2e  $\sigma$  bonds  
ON=1.71-1.77|e|



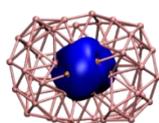
4\*5c-2e  $\pi$  bonds  
ON=1.78-1.81|e|



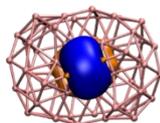
2\*19c-2e  $\pi$  bonds  
ON=1.88|e|



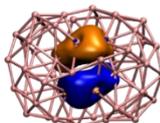
1\*52c-2e  $\pi$  bond  
ON=1.84|e|



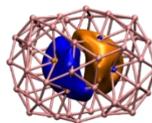
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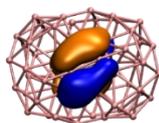
$P_y$



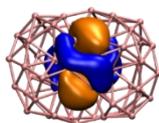
$P_z$



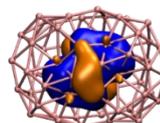
$P_x$



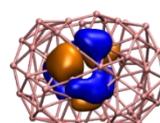
$D_{xz}$



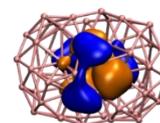
$D_{z^2}$



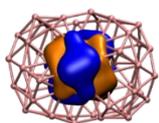
$D_{x^2-y^2}$



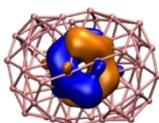
$D_{yz}$



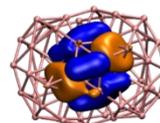
$D_{xy}$



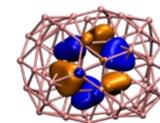
$F_{z(x^2-y^2)}$



$F_{xyz}$



$F_{yz^2}$



$F_{xz^2}$

13\*12c-2e  $\sigma$  bonds  
ON=1.52-2.00|e|

Table S1. The Cartesian coordinates of global minimum structures of neutral  $B_n$  ( $n = 52-64$ ) clusters.

B52-I	X	Y	Z
B	3.195754	0.794203	1.069776
B	1.596123	0.445824	1.607836
B	0.330057	1.414332	0.839399
B	1.214753	-1.178770	1.791381
B	2.774849	-0.790484	0.927074
B	-0.734420	2.731223	1.587371
B	2.421536	-2.372854	1.418883
B	-0.330057	-1.414332	0.839399
B	-1.596123	-0.445824	1.607836
B	-2.090536	-2.052443	1.386620
B	-0.890827	-3.142841	1.331180
B	-3.195754	-0.794203	1.069776
B	-2.421536	2.372854	1.418883
B	-2.774849	0.790484	0.927074
B	2.090536	2.052443	1.386620
B	0.734420	-2.731223	1.587371
B	-1.214753	1.178770	1.791381
B	0.000000	0.000000	1.871659
B	3.195754	0.794203	-1.069776
B	1.596123	0.445824	-1.607836
B	0.330057	1.414332	-0.839399
B	1.214753	-1.178770	-1.791381
B	2.774849	-0.790484	-0.927074
B	-0.734420	2.731223	-1.587371
B	2.421536	-2.372854	-1.418883
B	-0.330057	-1.414332	-0.839399
B	-1.596123	-0.445824	-1.607836
B	-2.090536	-2.052443	-1.386620
B	-0.890827	-3.142841	-1.331180
B	-3.195754	-0.794203	-1.069776
B	-2.421536	2.372854	-1.418883
B	-2.774849	0.790484	-0.927074
B	2.090536	2.052443	-1.386620
B	0.734420	-2.731223	-1.587371
B	-1.214753	1.178770	-1.791381
B	0.000000	0.000000	-1.871659
B	-0.965412	-4.419272	0.000000
B	-2.241729	-3.392501	0.000000
B	-3.248151	-2.110689	0.000000
B	0.965412	4.419272	0.000000
B	2.241729	3.392501	0.000000

B	3.248151	2.110689	0.000000
B	0.890827	3.142841	-1.331180
B	0.890827	3.142841	1.331180
B	1.912192	-3.829386	0.877655
B	1.912192	-3.829386	-0.877655
B	0.342051	-4.300081	1.086905
B	0.342051	-4.300081	-1.086905
B	-1.912192	3.829386	0.877655
B	-0.342051	4.300081	1.086905
B	-1.912192	3.829386	-0.877655
B	-0.342051	4.300081	-1.086905
B54-I	X	Y	Z
B	0.926612	-0.030275	-3.309914
B	-0.926612	0.030275	-3.309914
B	0.016671	2.881578	-3.064880
B	-0.016671	-2.881578	-3.064880
B	1.115358	-1.673761	-3.294317
B	-1.115358	1.673761	-3.294317
B	1.078186	1.603641	-3.306554
B	-1.078186	-1.603641	-3.306554
B	0.884067	-0.732479	3.819969
B	-0.884067	0.732479	3.819969
B	-1.019412	-0.906079	3.799385
B	1.019412	0.906079	3.799385
B	0.108552	-2.179516	3.611375
B	-0.108552	2.179516	3.611375
B	1.294056	-1.633611	2.417713
B	-1.294056	1.633611	2.417713
B	0.039382	-2.959477	2.166911
B	-0.039382	2.959477	2.166911
B	-0.842095	-0.031128	2.116179
B	0.842095	0.031128	2.116179
B	-1.394948	-1.736909	2.412462
B	1.394948	1.736909	2.412462
B	-0.858671	-1.474881	-0.422089
B	0.858671	1.474881	-0.422089
B	-1.677551	-0.832436	-1.918776
B	1.677551	0.832436	-1.918776
B	-1.411310	-2.478854	-1.902764
B	1.411310	2.478854	-1.902764
B	0.075511	4.586436	-0.417806
B	-0.075511	-4.586436	-0.417806
B	-0.099849	-3.912614	-1.812435
B	0.099849	3.912614	-1.812435

B	-1.383170	2.514848	-1.877625
B	1.383170	-2.514848	-1.877625
B	1.671807	-0.869975	-1.908110
B	-1.671807	0.869975	-1.908110
B	-1.221182	3.397024	-0.507398
B	1.221182	-3.397024	-0.507398
B	-0.832380	1.467077	-0.415861
B	0.832380	-1.467077	-0.415861
B	-1.894836	0.004209	-0.485306
B	1.894836	-0.004209	-0.485306
B	-1.383170	-3.363900	-0.509728
B	1.383170	3.363900	-0.509728
B	-1.758306	-0.880418	0.962253
B	1.758306	0.880418	0.962253
B	-1.780759	0.870424	0.976275
B	1.780759	-0.870424	0.976275
B	1.461265	2.555491	0.949026
B	-1.461265	-2.555491	0.949026
B	1.368448	-2.509340	0.969783
B	-1.368448	2.509340	0.969783
B	-0.428440	4.010451	0.952232
B	0.428440	-4.010451	0.952232
B56-I	X	Y	Z
B	-1.235729	1.609303	2.174591
B	-1.235562	1.078157	-2.479083
B	-1.235742	-2.688714	0.306456
B	3.539507	-0.975319	-1.368325
B	3.538937	-0.697072	1.528612
B	3.539794	1.671116	-0.160401
B	-2.945094	1.139228	-1.976316
B	-2.944855	-2.282154	0.001109
B	-2.944437	1.141684	1.974521
B	-1.235986	2.686021	-0.333458
B	-1.234772	-1.630934	-2.157617
B	-1.235206	-1.053312	2.491449
B	2.074318	1.651799	2.168489
B	2.074445	1.052726	-2.515442
B	2.074674	-2.704866	0.346600
B	1.331171	0.371200	3.117766
B	1.331110	2.515268	-1.881315
B	1.331799	-2.886484	-1.238200
B	-0.294521	-2.761233	-1.183336
B	-0.294903	0.355353	2.982345
B	-0.295192	2.406267	-1.798334

B	2.911009	0.315018	2.648819
B	2.910252	2.135225	-1.596015
B	2.910655	-2.449711	-1.050279
B	-1.955833	0.356798	2.995349
B	-1.956257	2.415555	-1.806397
B	-1.955614	-2.772519	-1.188908
B	0.443557	1.819658	-0.222922
B	0.446618	-1.103427	-1.462896
B	0.445316	-0.715620	1.685818
B	0.445367	1.091893	1.471136
B	0.446192	0.729228	-1.680889
B	0.444099	-1.820940	0.209964
B	2.073899	-1.096589	2.495653
B	2.074168	2.711252	-0.298331
B	2.074676	-1.613434	-2.198483
B	-0.475206	-2.315121	1.731196
B	-0.475589	2.657220	1.139320
B	-0.474314	-0.341542	-2.868910
B	-3.935492	0.116628	0.982409
B	-3.937413	0.791899	-0.592791
B	-3.937269	-0.910033	-0.390121
B	1.251913	2.726122	1.168560
B	1.252462	-0.350290	-2.945584
B	1.251986	-2.375845	1.775987
B	-2.945779	2.218586	-0.534815
B	-2.944577	-1.572096	-1.653966
B	-2.944159	-0.646252	2.187663
B	-3.844469	-1.530050	1.143691
B	-3.845149	1.755114	0.752434
B	-3.844890	-0.226364	-1.896678
B	3.538973	1.036233	1.322340
B	3.539414	0.626933	-1.558566
B	3.539923	-1.661887	0.235962
B	2.804021	0.000219	0.000373
B	0.963752	0.000103	-0.000231
B56-II	X	Y	Z
B	0.179417	-3.647923	1.053527
B	0.112196	-2.048699	1.656068
B	1.311932	-0.967852	0.841365
B	-1.410087	-1.339318	1.768789
B	-1.312019	-2.963319	0.961917
B	2.889943	-0.192225	1.425231
B	-2.800980	-2.336813	1.386759
B	-1.352423	0.257778	0.847710

B	-0.199355	1.282416	1.718944
B	-1.724538	2.049729	1.373624
B	-2.999519	1.050579	1.295094
B	-0.308348	2.942173	1.324500
B	2.767891	1.490783	1.401107
B	1.103368	1.956344	0.841966
B	1.591679	-2.733765	1.381738
B	-2.872525	-0.608346	1.578853
B	1.388405	0.532634	1.753214
B	-0.035808	-0.384084	1.902881
B	0.207903	-3.639799	-1.092930
B	0.129101	-2.038059	-1.676449
B	1.308853	-0.960587	-0.834859
B	-1.397443	-1.331689	-1.764963
B	-1.289443	-2.963360	-0.982532
B	2.866963	-0.172574	-1.358682
B	-2.784366	-2.337402	-1.385143
B	-1.346602	0.262646	-0.846691
B	-0.209999	1.289815	-1.704996
B	-1.732774	2.066002	-1.382428
B	-3.003505	1.068822	-1.315119
B	-0.317362	2.971205	-1.356033
B	2.719112	1.516250	-1.305260
B	1.081409	1.974920	-0.832981
B	1.612682	-2.723358	-1.398014
B	-2.858362	-0.601065	-1.573536
B	1.399580	0.550575	-1.770773
B	-0.025487	-0.373037	-1.910213
B	-4.263591	1.362913	0.002127
B	-3.046530	2.469759	0.022348
B	-1.606713	3.296409	0.008778
B	4.158401	-2.385335	0.038546
B	4.177724	-0.852261	-0.234987
B	3.798058	0.733573	-0.000768
B	2.912666	-3.318380	0.038863
B	1.434115	-3.976758	-0.003639
B	3.023571	-1.875963	-1.235923
B	3.014186	-1.865943	1.314385
B	-4.157891	-1.583906	0.874286
B	-4.146059	-1.582203	-0.877741
B	-4.346792	0.043383	1.077044
B	-4.333285	0.043053	-1.083537
B	-0.262561	4.246548	0.039555
B	1.038638	3.874164	-0.988000

B	2.583438	3.104271	1.032665
B	3.706613	2.373069	-0.058568
B	2.523988	3.172024	-0.916155
B	1.102535	3.822184	0.929038
B58-I	X	Y	Z
B	2.738132	1.810770	-0.618517
B	0.198205	-3.276318	-0.615904
B	-2.937358	1.464166	-0.617758
B	-2.196754	-3.122944	1.035009
B	-1.607198	3.465109	1.032693
B	3.805004	-0.340320	1.033337
B	-0.205238	3.372236	1.990908
B	3.021022	-1.506448	1.991948
B	-2.816543	-1.861035	1.992633
B	3.065828	-2.440834	-0.759123
B	-3.647676	-1.433955	-0.757892
B	0.581376	3.873964	-0.760522
B	3.794366	-0.981451	-0.759077
B	-2.747017	-2.793936	-0.758437
B	-1.047110	3.774550	-0.760593
B	1.543657	2.766824	-1.436425
B	1.623748	-2.721100	-1.430547
B	-3.168879	-0.048337	-1.435816
B	-3.378506	0.826669	0.970258
B	2.404149	2.512485	0.968291
B	0.974241	-3.336504	0.969330
B	2.561221	-2.834954	1.035531
B	-3.735762	-0.799195	1.034469
B	1.174957	3.635005	1.032762
B	3.253140	1.230224	0.969301
B	-0.561232	-3.430828	0.970508
B	-2.691847	2.202412	0.969312
B	-1.283411	-2.898718	-1.432916
B	-1.868445	2.559235	-1.436149
B	3.151136	0.337288	-1.434005
B	3.825676	-1.908682	0.676019
B	-3.565866	-2.358531	0.676591
B	-0.259796	4.266874	0.672639
B	1.426456	0.944224	1.499324
B	0.103446	-1.705502	1.501039
B	-1.529660	0.764650	1.498623
B	-1.706157	-1.129440	-0.895187
B	-0.124794	2.041330	-0.896297
B	1.831905	-0.913702	-0.895489

B	-0.061203	1.010054	0.469622
B	0.906263	-0.451669	0.470146
B	-0.843725	-0.557685	0.469429
B	-0.105430	1.739372	2.225059
B	1.557485	-0.775869	2.226755
B	-1.452067	-0.958508	2.226421
B	2.382509	1.575229	-2.218258
B	0.173618	-2.853728	-2.217237
B	-2.555506	1.273915	-2.217357
B	-1.679415	-0.150101	-2.441504
B	0.710789	1.524484	-2.438510
B	0.966664	-1.380680	-2.438375
B	0.055957	-0.919345	3.072242
B	-0.825880	0.414201	3.070745
B	0.769992	0.511135	3.071256
B	1.684233	0.055907	-2.440781
B	-0.791158	-1.487575	-2.439134
B	-0.891438	1.427305	-2.440551
B	-0.000102	-0.001724	-2.829840
B60-I	X	Y	Z
B	-4.061942	0.287966	1.156165
B	-2.454503	3.115900	-1.212490
B	-2.502449	-2.624641	1.436145
B	0.827416	3.210202	-1.431979
B	-1.508635	-1.018901	-0.827528
B	-0.000040	1.510466	0.841359
B	-0.827399	3.210071	-1.431963
B	-3.271909	-1.169013	1.455637
B	-0.000043	1.507388	-0.877731
B	-1.513880	-1.036730	0.876082
B	-4.072774	0.259648	-1.103283
B	-2.455895	3.129187	1.154222
B	-3.919883	-2.427695	0.125766
B	-0.000045	4.253723	-0.026368
B	-3.252216	1.708939	0.905952
B	-3.256090	1.699892	-0.914848
B	-2.548214	-2.647889	-1.255593
B	0.821911	3.213467	1.376169
B	-4.489710	-0.900925	0.046941
B	-1.592586	4.016766	-0.028453
B	-3.284156	-1.185677	-1.364699
B	-0.822002	3.213423	1.376162
B	-1.610232	1.751428	1.604444
B	-2.505969	0.246859	-1.706130

B	-2.489901	0.276337	1.722925
B	-1.616936	1.731869	-1.631713
B	-0.850697	0.273282	-1.909584
B	-0.840989	0.280686	1.892958
B	-3.023515	-3.685719	0.093632
B	1.592499	4.016811	-0.028425
B	3.271773	-1.168961	1.455509
B	2.548307	-2.647819	-1.255674
B	2.489838	0.276369	1.723008
B	0.853330	-2.604524	-1.381170
B	3.284183	-1.185575	-1.364674
B	2.502342	-2.624702	1.435925
B	3.252164	1.708986	0.906075
B	4.061895	0.288009	1.156256
B	1.508692	-1.018827	-0.827496
B	1.513812	-1.036668	0.876083
B	2.505987	0.246960	-1.706090
B	0.845007	-2.652544	1.497207
B	0.850722	0.273343	-1.909538
B	-0.000017	-1.194911	1.688630
B	0.000043	-1.190880	-1.686469
B	0.840900	0.280713	1.892991
B	-0.845106	-2.652510	1.497214
B	1.616916	1.731921	-1.631530
B	1.610144	1.751453	1.604472
B	-0.853142	-2.604595	-1.381124
B	2.455814	3.129212	1.154217
B	3.023866	-3.685729	0.093521
B	3.920087	-2.427611	0.125773
B	4.489754	-0.900797	0.047014
B	0.000013	-3.588594	-0.113056
B	1.586579	-3.897205	-0.489933
B	-1.586439	-3.897389	-0.490465
B	3.256060	1.699977	-0.914731
B	4.072777	0.259772	-1.103232
B	2.454481	3.116003	-1.212485
B62-I	X	Y	Z
B	3.848154	-1.507497	-1.131528
B	3.729360	1.727748	1.205593
B	1.078197	-3.290355	-1.313081
B	0.913145	3.365687	1.434914
B	0.931500	-1.469561	0.966359
B	0.799838	1.476513	-0.760108
B	2.310218	2.509110	1.495761

B	2.471714	-2.424804	-1.313792
B	0.843970	1.520119	0.967714
B	0.883570	-1.429848	-0.761875
B	3.822705	-1.513545	1.205141
B	3.756207	1.721163	-1.128148
B	2.376668	-3.794087	-0.051883
B	2.158258	3.922476	-0.052476
B	3.855891	0.108353	-1.009765
B	3.820978	0.108299	0.855713
B	1.103798	-3.307489	1.435078
B	0.889868	3.343859	-1.312481
B	3.608899	-2.744790	0.036814
B	3.448197	2.944899	0.038125
B	2.450447	-2.374506	1.494877
B	2.329893	2.558566	-1.311268
B	2.365520	0.936874	-1.649074
B	2.383084	-0.750555	1.656940
B	2.414922	-0.803002	-1.649948
B	2.335943	0.884175	1.656525
B	1.001075	0.027858	-1.841627
B	0.907181	-4.448707	0.053378
B	0.653732	4.491931	0.052054
B	-3.359321	0.716315	-1.386333
B	-3.383011	-0.911373	1.398703
B	-1.982971	1.593702	-1.684855
B	-1.866116	-1.635751	1.653979
B	-3.430475	0.720903	1.398113
B	-3.311562	-0.905943	-1.385196
B	-1.981965	3.211926	-0.931649
B	-1.796148	-3.319820	-0.928610
B	-3.230184	-2.567347	-1.103295
B	-3.371213	2.379844	-1.107204
B	-1.660169	-0.046278	0.872739
B	-1.707715	-0.048304	-0.834436
B	-1.956898	1.530117	1.652873
B	-1.888726	-1.705185	-1.683442
B	-0.496346	0.787079	2.001522
B	-0.452431	-0.858859	-1.824147
B	-0.449711	-0.811608	2.001044
B	-0.500358	0.830760	-1.824377
B	-0.355354	-2.518017	-1.626702
B	-0.470565	2.413153	1.671354
B	-0.497161	2.492537	-1.628515
B	-0.331136	-2.433550	1.671894

B	-0.371796	-4.097885	-0.964873
B	-0.603722	4.068735	-0.965813
B	-4.180496	-1.718021	-0.020846
B	-4.448457	-0.125897	-0.126487
B	-4.271220	1.478924	-0.022773
B	-1.771752	-3.296544	0.913516
B	-3.189999	-2.524238	1.150767
B	-0.329438	-4.052583	1.169712
B	-1.957279	3.193157	0.910678
B	-3.329239	2.342008	1.148256
B	-0.559997	4.029158	1.166472
B64-1	X	Y	Z
B	-1.338228	0.564335	1.415872
B	-1.338228	0.564335	-1.415872
B	-3.070455	-0.166113	1.789048
B	-3.070455	-0.166113	-1.789048
B	2.427829	1.364976	-1.800628
B	2.427829	1.364976	1.800628
B	2.407428	-0.045005	0.827847
B	2.407428	-0.045005	-0.827847
B	-0.932241	3.863368	1.397482
B	-0.932241	3.863368	-1.397482
B	3.502292	-1.313475	-1.641007
B	3.502292	-1.313475	1.641007
B	-0.261791	0.279040	3.374394
B	-0.261791	0.279040	-3.374394
B	2.134212	2.777087	1.065378
B	2.134212	2.777087	-1.065378
B	-2.217807	-2.903424	-1.302023
B	-2.217807	-2.903424	1.302023
B	-3.317111	-1.579065	-0.772323
B	-3.317111	-1.579065	0.772323
B	-3.016646	1.236084	-0.957099
B	-3.016646	1.236084	0.957099
B	-1.571980	-0.577696	2.741773
B	-1.571980	-0.577696	-2.741773
B	-0.264675	-1.391899	3.510248
B	-0.264675	-1.391899	-3.510248
B	-2.774907	-1.714990	-2.321119
B	-2.774907	-1.714990	2.321119
B	2.659496	-0.175551	-2.609197
B	2.659496	-0.175551	2.609197
B	0.935926	-2.480710	0.836163
B	0.935926	-2.480710	-0.836163

B	-0.590390	-3.146393	1.291413
B	-0.590390	-3.146393	-1.291413
B	-0.491992	2.978224	-2.607561
B	-0.491992	2.978224	2.607561
B	1.204775	2.367299	-2.430869
B	1.204775	2.367299	2.430869
B	0.114109	1.863534	3.624236
B	0.114109	1.863534	-3.624236
B	1.179986	-0.740190	-3.288695
B	1.179986	-0.740190	3.288695
B	2.753237	-2.633132	-1.015471
B	2.753237	-2.633132	1.015471
B	-1.588315	2.285055	-1.156514
B	-1.588315	2.285055	1.156514
B	1.675288	-1.346639	-1.751176
B	1.675288	-1.346639	1.751176
B	0.739160	3.652244	1.478987
B	0.739160	3.652244	-1.478987
B	-1.274649	-2.351010	-2.627749
B	-1.274649	-2.351010	2.627749
B	1.463544	0.955913	-3.256923
B	1.463544	0.955913	3.256923
B	1.987616	-3.711328	0.000000
B	-0.551622	0.069246	-0.000000
B	-2.968549	2.612909	-0.000000
B	1.380967	3.764673	-0.000000
B	-1.510140	-3.744786	0.000000
B	-1.811776	3.770370	-0.000000
B	3.628502	-1.120661	0.000000
B	-2.313045	-0.171316	0.000000
B	0.300385	-3.911277	0.000000
B	0.885471	-0.801561	0.000000
B64-II	X	Y	Z
B	2.590145	-2.684632	-1.286999
B	-2.562313	1.654411	-2.495732
B	2.251855	-1.881156	-2.729585
B	-2.240240	0.220176	-3.310407
B	0.641934	0.559057	-2.860570
B	-0.615721	-1.945989	-2.182409
B	3.051134	-0.090755	2.100927
B	-3.066448	1.159121	1.727126
B	0.782880	3.231803	1.769966
B	-0.805975	-1.868749	3.179718
B	-4.297995	-0.266014	-0.808351

B	4.302086	-0.184745	-0.799638
B	3.260534	0.661954	-1.791629
B	-3.251462	-1.508352	-1.221130
B	-3.009614	2.618567	-1.222926
B	3.009731	-2.871912	0.320981
B	1.902876	1.551611	-2.481475
B	-1.889591	-2.601085	-1.342951
B	-0.822374	0.316580	-0.252738
B	0.810178	-0.389480	-0.056631
B	0.609120	1.015532	-1.052267
B	-0.612564	-1.415125	-0.387172
B	0.877916	-1.881627	-1.232915
B	-0.876731	0.988296	-2.030454
B	1.170850	1.893936	2.587423
B	-1.190627	-0.298725	3.182475
B	-0.131638	3.174409	-0.894661
B	0.145215	-3.198569	0.843240
B	-1.654959	1.300273	2.710839
B	1.633613	0.275816	2.996662
B	-3.825496	1.251240	-1.133337
B	3.846347	-1.650062	-0.321325
B	1.452533	-0.848149	1.501062
B	-1.460790	1.492673	0.852272
B	3.446772	1.493289	1.192592
B	-3.463629	-0.683067	1.763062
B	3.949012	1.411784	-0.411919
B	-3.952944	-1.428835	0.375465
B	1.424462	-3.207356	-0.195818
B	-1.412522	2.659854	-1.814700
B	-1.401243	-2.795328	0.383743
B	1.414393	2.606228	-1.104196
B	-3.343846	-0.154965	-2.170235
B	3.356274	-0.980772	-1.915109
B	0.519641	-2.349419	2.380494
B	-0.548023	3.240525	0.848917
B	2.354060	2.750597	1.714032
B	-2.365088	-1.489073	2.886176
B	3.149483	-1.462486	1.243810
B	-3.167693	1.880356	0.312207
B	-0.759818	-0.452504	-3.230182
B	0.790458	-1.266104	-3.000687
B	1.656443	-0.299207	-1.692323
B	-1.652000	-0.617744	-1.622388
B	0.436236	-0.800179	3.208233

B	-0.459047	2.341003	2.344520
B	1.766102	-2.624891	1.421930
B	-1.763544	2.986987	-0.112642
B	-2.786778	0.144601	2.997115
B	2.762566	1.409607	2.658159
B	2.700249	2.482540	0.052578
B	-2.688924	-2.110205	1.295065
B	3.033515	2.326034	-1.541277
B	-3.018973	-2.791599	-0.144013