

Electronic Supplementary Information (ESI)
**Formation of the quasi-planar B₅₆ boron cluster: topological path
from B₁₂ and disk aromaticity**

Fernando Buendía,^a Hung Tan Pham,^b José Enrique Barquera-Lozada,^c

Marcela Beltrán Sanchez^d and Minh Tho Nguyen^{b,e,*}

^a Instituto de Física, Universidad Nacional Autónoma de México, C.P. 04510 Cd. de México, México

^b Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium.

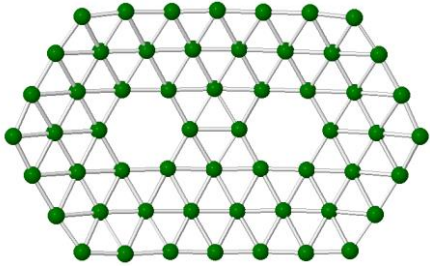
^c Instituto de Química, Universidad Nacional Autónoma de México, Ciudad de México, 04510 México

^d Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México,
C.P. 04510 Cd. de México, México

^e Institute for Computational Science and Technology (ICST), Ho Chi Minh City, Vietnam.

* Email: minh.nguyen@kuleuven.be

Table 1. Cartesian coordinates of the most stable isomers A-J of B₅₆ optimized at the TPSSh/6-311+G(d) level.

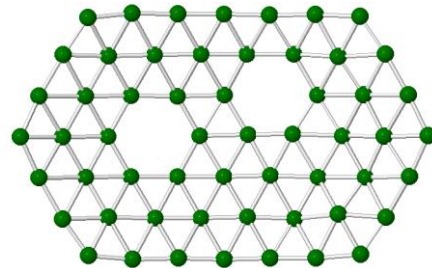
B56			
#Energy = 0.0 eV (A)			
B	0.900106	0.002507 -0.866462	
B	-0.870274	-0.001793 -0.886862	
B	0.017286	-1.453923 -0.862002	
B	0.010846	1.455407 -0.889522	
B	1.699516	-1.433253 -0.751842	
B	1.694466	1.442507 -0.776962	
B	-1.667774	-1.440903 -0.797562	
B	-1.674744	1.434007 -0.818852	
B	0.849176	-2.912253 -0.436162	
B	-0.819884	-2.917053 -0.459802	
B	0.836756	2.921297 -0.477042	
B	-0.834904	2.916777 -0.496402	
B	3.354036	-1.443973 -0.525692	
B	3.348436	1.454797 -0.542002	
B	-3.327884	-1.458263 -0.621652	
B	-3.334644	1.440087 -0.639102	
B	2.498056	-2.886303 -0.265312	
B	2.488246	2.899717 -0.298382	
B	-2.472954	-2.892473 -0.322222	
B	-2.487914	2.884887 -0.358012	
B	4.180156	0.006477 -0.422542	
B	-4.162074	-0.012273 -0.544932	
B	0.010026	-4.337213 0.073518	
B	-0.009554	4.345197 0.025308	
B	1.637026	-4.296053 0.153848	
B	-1.618544	-4.298983 0.117408	
B	1.619236	4.309227 0.109358	
B	-1.639294	4.299987 0.070208	
B	4.133986	-2.858763 0.073068	
B	4.120626	2.874397 0.055598	
B	-4.120064	-2.874293 -0.043642	
B	-4.132864	2.855557 -0.064292	
B	4.960116	-1.430503 -0.004592	
B	4.948656	1.445607 0.000218	
B	-4.951754	-1.452433 -0.158852	
B	-4.952734	1.424057 -0.154802	
B	3.262086	-4.305223 0.459238	
B	3.241296	4.321717 0.429798	
B	-3.252584	-4.313253 0.379468	
B	-3.270754	4.303687 0.342098	
B	5.754696	0.009577 0.255548	
B	-5.761324	-0.014223 0.071668	
B	4.793286	-4.155403 0.861468	
B	4.770786	4.173807 0.846458	
B	-4.798224	-4.169763 0.728208	

B	-4.813514	4.150277	0.705248
B	5.697826	-2.859743	0.757328
B	5.678146	2.880077	0.756818
B	-5.708754	-2.881193	0.582008
B	-5.715974	2.855047	0.577908
B	6.512646	1.435077	0.864458
B	6.522546	-1.410583	0.861068
B	-6.547994	-1.438143	0.644978
B	-6.549744	1.408397	0.647778
B	7.151916	0.013407	1.140508
B	-7.195284	-0.015343	0.894928

B56

#Energy=+1.12 eV (B)

B	-4.167294	-0.002512	-0.497311
B	-1.683104	-1.446774	-0.846668
B	-3.341419	-1.447742	-0.601263
B	-4.949369	-1.439219	-0.114820
B	-0.873674	0.019869	-0.888668
B	-5.758820	-0.008129	0.141960
B	-0.015589	-1.466146	-0.894613
B	-0.824434	-2.901468	-0.475679
B	-2.469641	-2.879177	-0.296324
B	-4.118980	-2.855970	0.018740
B	2.460768	0.062865	-0.646097
B	0.820295	2.922853	-0.530174
B	2.480722	2.915161	-0.397903
B	4.085262	2.816709	0.131140
B	-0.834320	2.921274	-0.441582
B	-2.482014	2.885236	-0.280268
B	-4.126347	2.859923	0.025788
B	0.005609	1.479768	-0.914640
B	3.342111	1.456178	-0.570406
B	4.986642	1.447656	-0.087566
B	-1.681967	1.444275	-0.756100
B	-3.334908	1.453091	-0.578571
B	-4.954975	1.438025	-0.106184
B	0.853368	0.038412	-0.918390
B	4.212905	0.011471	-0.549685
B	5.716553	-0.024609	0.279035
B	1.670995	-1.420521	-0.793604
B	3.365518	-1.477680	-0.670813
B	5.012802	-1.472939	-0.216599
B	0.828616	-2.884323	-0.355640
B	2.494530	-2.930490	-0.369934
B	4.066790	-2.781097	0.205502
B	-7.184338	-0.010891	0.982236
B	7.204255	-0.020895	0.980128
B	6.533973	1.411701	0.752571
B	-6.537750	1.412921	0.730515
B	6.561903	-1.442070	0.725064

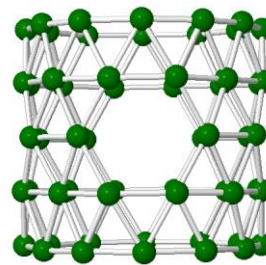


B	-6.544107	-1.431499	0.726183
B	5.719722	2.853735	0.648810
B	-5.707247	2.858913	0.661193
B	5.716858	-2.869856	0.627396
B	-5.699284	-2.870262	0.667785
B	1.619637	4.254411	0.163486
B	3.249421	4.261033	0.398726
B	-0.004179	4.305820	0.080588
B	-1.643854	4.305318	0.151295
B	-3.271101	4.324779	0.440994
B	-4.809668	4.157490	0.800090
B	4.808869	4.148748	0.771757
B	1.623048	-4.303659	0.141193
B	3.248836	-4.288158	0.435548
B	-0.000589	-4.349400	0.091199
B	-1.615208	-4.289316	0.166125
B	-3.242128	-4.292273	0.436952
B	-4.786360	-4.152031	0.800966
B	4.801741	-4.155035	0.767079

B56

#Energy = +1.13 eV (C)

B	-2.895244	-1.448472	-0.733631
B	-1.165154	0.147468	-3.110251
B	-0.272944	0.694098	3.449819
B	-2.736134	-1.790062	0.946109
B	1.098556	1.551938	3.047419
B	0.316666	1.016138	-3.233471
B	1.162516	-0.148412	3.106989
B	-0.319734	-1.015362	3.231989
B	-2.025264	-2.813012	-0.235441
B	-3.489064	-0.338172	0.405879
B	0.271706	-0.691742	-3.448081
B	-1.131304	1.803368	-2.750111
B	2.906326	1.448878	0.734719
B	1.124916	-1.800872	2.738319
B	-1.567994	-2.939322	1.392499
B	-1.990734	-2.377682	-1.841061
B	-1.098204	-1.553952	-3.051181
B	2.738516	1.790498	-0.944491
B	-2.934394	-0.467332	2.006929
B	-0.376854	-2.555732	2.518829
B	-2.512184	0.931908	-2.420341
B	-3.389064	0.113138	-1.196011
B	1.747336	0.092358	-3.131881
B	-0.306064	2.363488	3.575979
B	0.369046	2.553548	-2.508821
B	3.492056	0.336848	-0.408171
B	2.032076	2.814178	0.239589
B	2.936696	0.470178	-2.008511
B	2.508316	-0.934512	2.414569

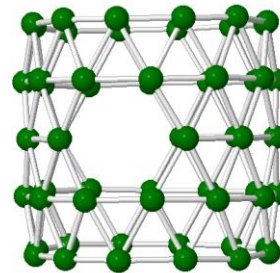


B	1.560806	2.935508	-1.382751
B	3.394126	-0.116102	1.193709
B	2.000476	2.375948	1.844809
B	-1.747994	-0.084892	3.128859
B	-3.052434	0.948518	2.903539
B	-1.013664	-4.114232	0.229199
B	-0.758294	-3.195002	-2.704391
B	-3.857924	0.917488	1.508679
B	1.720326	-1.598572	-3.535571
B	1.103076	-3.434472	2.229079
B	-3.591124	1.797328	-1.413341
B	-1.294704	-3.850282	-1.331001
B	0.309156	-2.360512	-3.580861
B	-1.111144	3.432068	-2.223461
B	-4.149254	1.129458	-0.054931
B	-1.720084	1.605958	3.525949
B	-2.503454	2.631918	-2.261721
B	-0.299374	-4.001002	1.669129
B	3.859186	-0.916602	-1.513291
B	2.494436	-2.634112	2.253619
B	3.586606	-1.801162	1.406169
B	3.049206	-0.943822	-2.906351
B	1.014506	4.113098	-0.218511
B	0.768506	3.194668	2.708149
B	0.286036	3.995838	-1.650751
B	4.148936	-1.132752	0.049849
B	1.309686	3.852308	1.338039

B56

#Energy = +1.17 eV (D)

B	-1.253779	3.010616	0.348390
B	1.948451	2.592996	0.083850
B	-2.624599	1.977886	0.357620
B	2.890301	1.197476	-0.102820
B	-0.564169	3.374296	-1.163980
B	-3.151449	-1.305864	0.110000
B	-1.873219	2.402876	1.842490
B	-3.372329	-0.315504	-1.217580
B	2.620331	1.835096	1.486130
B	-2.096509	2.670996	-1.121800
B	3.215781	-0.457924	-0.267350
B	-3.162689	1.388166	-1.146000
B	-2.944749	1.125016	1.797790
B	-0.462969	-3.253914	-0.248480
B	-0.349879	3.118516	1.787400
B	3.058181	0.517576	-1.687730
B	1.108431	3.136996	-1.294460
B	1.323441	2.890156	1.638310
B	-3.164509	-0.565334	1.606050
B	-2.522279	-2.126214	1.423640
B	2.399711	2.087686	-1.506310

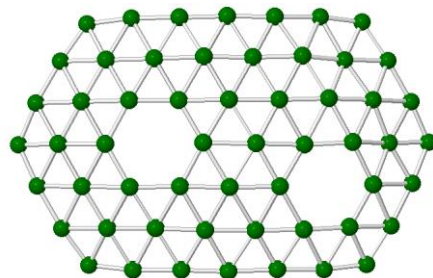


B	1.231241	-3.018364	-0.346800
B	2.068221	-2.750524	1.112440
B	-2.723359	-1.876754	-1.399060
B	3.273261	0.261756	1.305290
B	0.274461	-3.067654	-1.784240
B	2.887281	-1.149004	-1.786800
B	3.093791	-1.401014	1.145220
B	1.861031	-2.498574	-1.838990
B	-1.379729	-2.917824	-1.644370
B	-1.170239	-3.177484	1.298030
B	0.486291	-3.327434	1.179590
B	-1.405939	3.113026	-2.628670
B	-3.335049	0.642776	-2.666080
B	-2.274389	1.590766	3.280870
B	0.587741	2.880906	3.183880
B	1.630991	2.696796	-2.865100
B	-2.707879	2.113306	-2.607350
B	0.162631	3.386996	-2.699250
B	-0.974839	2.591266	3.290920
B	2.059131	2.198496	3.022080
B	-2.741059	-1.473804	2.968650
B	3.001321	0.899146	2.896520
B	2.825531	-0.175894	-3.194970
B	2.570691	1.409996	-3.096400
B	-3.148169	-0.967724	-2.761310
B	-2.911449	0.127976	3.177370
B	-2.143899	-2.223224	-2.996820
B	0.957611	-2.603944	-3.288250
B	2.683891	-2.208294	2.597760
B	-1.731909	-2.739874	2.843290
B	-0.251319	-3.326994	2.711960
B	-0.666939	-2.808474	-3.176350
B	2.274771	-1.708224	-3.282440
B	3.240951	-0.679284	2.691350
B	1.373821	-3.114434	2.632880

B56

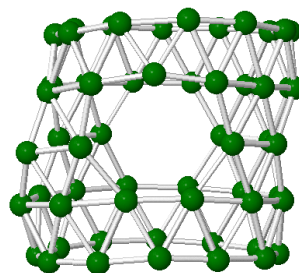
#Energy=+1.38 eV (E)

B	-2.544516	-0.075998	-0.670008
B	-4.208975	0.002775	-0.520596
B	-1.676899	-1.474745	-0.803219
B	-4.974340	-1.447659	-0.127373
B	-0.877928	-0.021227	-0.919214
B	-5.695019	0.003553	0.287798
B	0.026958	-1.488573	-0.891390
B	-0.860325	-2.944872	-0.427885
B	-2.501966	-2.933823	-0.366573
B	-4.131935	-2.868961	-0.014402
B	0.830897	2.901012	-0.476240
B	2.488359	2.866637	-0.292437
B	4.133851	2.859984	-0.004005

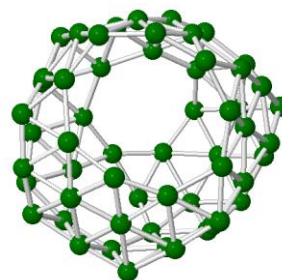


B	-0.848125	2.889542	-0.403227
B	-2.500463	2.917122	-0.368916
B	-4.101490	2.860548	0.129633
B	0.019438	1.446448	-0.908514
B	1.692105	1.434244	-0.787806
B	3.360862	1.455508	-0.602949
B	4.964144	1.443030	-0.087885
B	-1.689554	1.447978	-0.818539
B	-3.383307	1.465722	-0.597109
B	-5.018238	1.473248	-0.118681
B	0.884956	0.001025	-0.872097
B	4.174157	0.002328	-0.497688
B	5.777516	0.011504	0.137199
B	1.683270	-1.448975	-0.792976
B	3.348815	-1.452814	-0.592985
B	4.975993	-1.431896	-0.101448
B	0.832439	-2.931959	-0.468264
B	2.497828	-2.868694	-0.271765
B	4.129869	-2.847992	-0.003014
B	-7.203270	0.027829	0.961181
B	7.195984	0.017738	0.985473
B	6.557650	1.434400	0.730035
B	-6.559246	1.453333	0.714880
B	6.547353	-1.411222	0.725239
B	-6.519979	-1.392008	0.716253
B	5.713738	2.867025	0.678157
B	-5.722137	2.873049	0.663000
B	5.721466	-2.847813	0.654228
B	-5.682148	-2.837053	0.652481
B	1.623170	4.273571	0.151195
B	3.251559	4.281680	0.435431
B	0.002410	4.308574	0.086009
B	-1.634350	4.285719	0.132477
B	-3.267057	4.323829	0.433265
B	-4.802536	4.186774	0.794494
B	4.789145	4.143952	0.812710
B	1.632312	-4.292875	0.155748
B	3.269811	-4.285906	0.432805
B	0.017244	-4.341988	0.104090
B	-1.636848	-4.289387	0.140386
B	-3.270660	-4.288675	0.427923
B	-4.802788	-4.141451	0.810952
B	4.809794	-4.133533	0.801210
B56			
#Energy = +2.07 eV (F)			
B	-3.012911	-0.851774	0.601768
B	-2.048261	-2.220484	0.991888
B	-2.508421	2.220186	-0.649732
B	-1.076921	3.049656	-1.133222
B	-1.937531	2.079326	-2.257302

B	-2.800571	-2.128364	-0.552282
B	2.969909	0.863706	-0.479662
B	1.981229	-2.624754	0.828288
B	-1.587441	3.138186	0.467208
B	-2.752951	2.036466	1.007918
B	-2.219511	-0.950374	2.099268
B	2.075859	2.218246	-1.020772
B	-3.060471	0.953816	-1.666962
B	1.408989	-3.503814	-0.419372
B	-2.935501	0.499066	1.623578
B	-0.092721	3.763596	0.070658
B	-3.383751	-0.597094	-1.042262
B	-1.725591	-3.357074	-0.232792
B	-0.207711	-4.157014	-0.170172
B	-0.356691	2.560626	-2.573982
B	-1.037141	-2.086044	2.363288
B	2.399789	0.948706	-2.090832
B	0.752199	-3.707384	1.090148
B	0.733849	-2.592304	2.325518
B	1.595909	3.387836	0.099958
B	1.273589	2.128486	-2.511112
B	2.523549	-1.885724	2.218428
B	3.500439	0.878546	1.149788
B	2.278419	-2.086484	-0.846912
B	2.772849	2.269856	0.528438
B	2.742009	-0.580934	-1.413792
B	3.406349	-0.538714	1.899768
B	-3.318721	-0.357564	-2.708542
B	-2.430171	-3.212044	-1.788332
B	-1.259141	1.722856	-3.762702
B	-1.969931	3.103376	2.143498
B	-2.586891	0.938326	-3.327222
B	-3.213631	-1.868274	-2.186672
B	0.537469	-4.150404	-1.734832
B	-2.341091	0.343006	3.252858
B	-0.752341	4.009696	1.632088
B	-2.752441	1.788386	2.669808
B	-1.415641	-0.934224	3.573318
B	-1.081041	-4.085124	-1.598342
B	0.849679	4.068216	1.474448
B	1.758149	0.959846	-3.649352
B	-0.034021	-1.761604	3.624878
B	1.781279	-3.218384	-2.085942
B	0.353729	1.736986	-3.876502
B	2.571269	-1.872424	-2.483432
B	1.581269	-1.726114	3.590398
B	2.391139	-0.415114	-3.129622
B	3.174679	2.243706	2.228408
B	2.789109	-0.710594	3.373728
B	3.367249	0.802326	2.843288



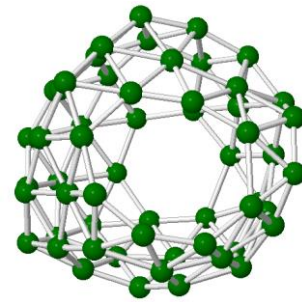
B	2.329229	3.467186	1.620018	
B56				
#Energy = +2.32 eV (G)				
B	-0.041374	2.728859	1.415629	
B	2.344976	-2.665821	-1.078171	
B	3.164546	-1.219561	-1.322771	
B	-0.365654	1.570469	2.531489	
B	-0.821194	3.136719	-1.293511	
B	-2.770074	-1.884221	0.624039	
B	2.820456	2.360449	0.771989	
B	-3.361164	-0.506851	-0.230841	
B	-1.611944	2.188749	1.575699	
B	1.687126	-1.511711	-2.145151	
B	3.489816	1.426079	-0.428531	
B	-0.157454	0.957059	-3.053841	
B	-1.294244	1.976549	-2.372191	
B	-2.384734	2.499359	-1.165771	
B	0.641876	0.217689	2.913279	
B	0.564416	-4.072301	0.763389	
B	3.117606	0.818979	1.202849	
B	-0.076144	3.658009	0.086139	
B	2.066456	-0.203491	2.153299	
B	-2.714924	-0.217471	-1.697221	
B	2.526096	-0.137211	-2.508471	
B	-1.793464	-2.667941	1.914689	
B	0.951606	-0.297531	-3.027281	
B	-3.506834	1.131259	-0.907631	
B	-1.536874	-1.312521	-2.295281	
B	0.258166	2.514749	-2.576411	
B	1.361786	3.077369	0.552479	
B	-4.019324	0.840779	0.634809	
B	-0.338564	-2.462511	2.938479	
B	2.407546	2.615649	-0.810621	
B	-1.639544	-1.311461	3.023859	
B	-3.766894	-0.599471	1.377939	
B	1.913776	-3.021481	0.570989	
B	3.901246	0.318989	-1.621221	
B	-1.818314	0.357719	-3.087781	
B	3.394066	-0.805481	1.324019	
B	-1.062154	0.244769	3.561619	
B	1.034596	-2.964921	1.956529	
B	1.153526	-3.860161	-0.715351	
B	0.951936	3.415959	-1.178321	
B	2.937646	1.552899	-2.140561	
B	-3.056144	-1.692811	2.274249	
B	0.088066	-1.841221	-2.779551	
B	-0.530504	-3.732491	1.908779	
B	1.149996	-1.425851	2.889909	
B	-2.467394	-1.710551	-1.011981	
B	-2.016634	1.389179	3.001269	



B	0.956726	-3.022471	-2.049021
B	-2.940184	1.381349	-2.398311
B	3.865626	-0.210591	-0.062421
B	1.896116	2.797209	-2.369651
B	-0.639224	-0.621461	-3.602041
B	-0.168604	-1.068451	3.842179
B	2.341766	-1.938791	1.815909
B	-3.165884	1.603619	1.894679
B	-2.922124	2.206359	0.409709

B56
#Energy = +2.36 eV (H)

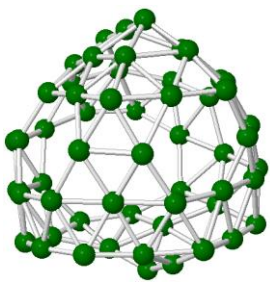
B	0.423822	2.691128	-1.757906
B	-0.901358	3.078197	-0.837736
B	1.936882	-1.049162	-2.531866
B	-1.894008	-1.423513	2.038574
B	-2.264608	0.239607	2.339334
B	-1.493448	-2.734933	0.838254
B	-0.877498	-0.499353	2.981094
B	1.978722	2.518788	0.486334
B	2.563622	0.304417	-1.659796
B	2.813052	1.627707	-0.642936
B	0.017742	-3.238853	0.316754
B	0.724442	2.969988	1.506964
B	-2.369128	2.261268	-0.974586
B	0.424022	-0.275472	-3.208846
B	-2.519768	0.904687	-1.968336
B	1.821052	0.567018	-3.173436
B	0.528802	-2.016522	-2.672056
B	0.406282	2.013518	2.803224
B	0.764562	3.562117	-0.247446
B	-2.347188	-0.675532	-2.512886
B	0.767392	-0.781632	3.163354
B	-0.916848	2.800617	1.994504
B	-1.254408	-3.216003	-0.837376
B	2.014692	2.137818	2.124454
B	-2.344538	1.902638	1.864334
B	2.060552	3.117698	-1.121736
B	1.517252	-2.800782	1.160454
B	3.583162	0.190618	-0.353476
B	-1.872988	2.967718	0.537014
B	0.082572	0.622378	3.625324
B	-3.492178	-1.819122	-1.670686
B	0.300972	-3.235333	-1.419496
B	1.942522	1.854938	-2.182456
B	2.453832	-0.569133	2.572994
B	2.952502	-1.235523	-1.149556
B	1.679862	0.784698	3.248634
B	-3.052548	-2.188382	1.076944
B	0.309752	1.367458	-2.730436
B	-3.402678	-0.759462	1.681134



B	-1.058918	0.429697	-2.703596
B	-0.545578	3.877838	0.715064
B	1.667392	-2.028993	2.568444
B	-2.488888	-2.995613	-2.001016
B	1.528752	-3.379263	-0.373746
B	2.933822	-1.763302	1.529264
B	-3.564288	1.058528	-0.628096
B	-3.479648	0.807818	1.281234
B	-0.911168	-1.216563	-3.203936
B	-3.339888	2.226207	0.484944
B	3.673862	-0.129272	1.372314
B	2.831422	-2.521992	-0.025816
B	-2.771488	-2.848533	-0.362086
B	-3.717768	-0.234633	-1.623516
B	-0.901998	-2.835163	-2.541666
B	3.130662	0.930907	2.526414
B	3.948822	-1.343972	0.279164

B56
#Energy = +2.39 eV (I)

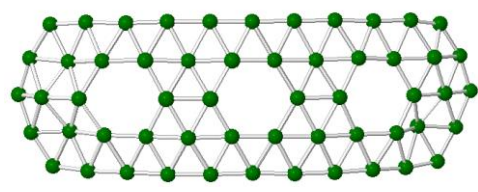
B	-0.644490	2.672360	1.078376
B	0.744650	2.989140	0.230606
B	-2.081450	2.170330	0.329176
B	0.911790	2.694960	1.856586
B	-2.076250	1.979360	-1.353554
B	-0.466220	2.099730	2.786506
B	0.691740	2.892290	-1.515284
B	-1.925800	2.161450	1.991886
B	-0.524840	-1.898420	2.634286
B	-0.065920	0.639540	3.549806
B	0.907810	-2.460960	1.805016
B	2.174030	2.718250	-0.688444
B	2.232480	2.793130	0.945876
B	-0.769160	2.465810	-2.330004
B	-3.259490	0.982950	-0.225504
B	2.202750	-2.258830	0.712846
B	-1.675560	1.068050	-2.669534
B	3.128760	-0.897580	0.972676
B	3.353430	0.219620	-0.316154
B	2.800880	-1.343430	-0.655884
B	-3.095180	1.300180	1.379286
B	0.686790	-3.067890	0.225596
B	-0.547180	-2.992020	1.326106
B	-1.975670	-2.372530	1.670736
B	1.017790	1.917790	3.370176
B	2.813830	-0.131090	-1.873014
B	1.755670	0.518220	3.582406
B	-3.605810	-0.222150	0.956696
B	1.818440	-2.634860	-0.956974
B	2.407810	-1.801850	2.270806
B	-3.054100	0.595520	-1.886284



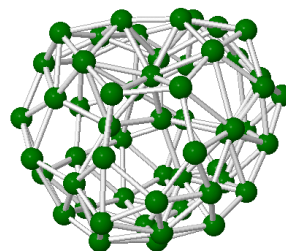
B	-0.880410	-0.780420	3.862016
B	3.600080	0.660910	1.306916
B	3.453810	1.907940	0.209276
B	3.040020	-0.120550	2.601166
B	0.794840	2.148690	-3.068044
B	3.206360	1.527890	-1.454414
B	1.699980	-0.602910	-3.008214
B	1.009660	-2.076480	-2.410174
B	-2.128260	-1.372510	3.079106
B	0.706850	-0.884340	3.949826
B	0.320580	-3.129990	-1.361244
B	-3.611610	-0.581690	-0.677864
B	2.138360	2.510790	-2.288404
B	0.599380	0.405620	-3.701134
B	0.154040	-1.181820	-3.445824
B	-3.343560	-2.025240	0.541216
B	-0.615830	-2.466270	-2.555844
B	-3.338160	-1.503150	2.051106
B	-2.195460	-2.135610	-2.271194
B	-0.535740	1.614640	-3.814204
B	-2.390790	-0.443000	-3.211884
B	2.313040	-1.014260	3.751346
B	-1.061310	0.057290	-3.977104
B	-3.328290	-2.228250	-1.070684
B	-3.489100	-1.084370	-2.240564

B56
#Energy= +2.56 eV (J)

B	1.658964	0.002882	0.049238
B	3.329031	0.005295	0.117614
B	6.686984	-0.010687	0.405937
B	8.246840	-0.009310	0.984399
B	9.450174	0.005919	2.155352
B	-1.662905	0.004476	0.027735
B	-3.330017	0.004311	0.105817
B	-6.546492	-0.013430	0.669253
B	-8.118183	-0.004385	1.250607
B	-9.582861	0.008635	1.988666
B	0.828437	1.463029	0.208346
B	2.477984	1.445739	0.396400
B	4.128707	1.475451	0.241946
B	5.773308	1.450564	0.447821
B	7.264668	1.372095	1.200031
B	8.888566	1.461209	1.841260
B	-0.820038	1.458514	0.236849
B	-2.473360	1.449472	0.385120
B	-4.124516	1.481596	0.310477
B	-5.722015	1.439839	0.732670
B	-7.406063	1.445313	0.702872
B	-8.972818	1.456823	1.682716
B	0.827051	-1.463053	0.135302



B	2.486748	-1.490705	0.108231	
B	4.111850	-1.457886	0.402630	
B	5.760291	-1.448265	0.521297	
B	7.231910	-1.358986	1.303410	
B	8.879209	-1.451704	1.876004	
B	-0.827364	-1.473076	0.072089	
B	-2.494652	-1.482492	0.092061	
B	-4.110945	-1.468607	0.383056	
B	-5.774403	-1.474558	0.512655	
B	-7.118452	-1.345266	1.536430	
B	-8.900690	-1.437923	1.856134	
B	0.006972	2.918299	0.431299	
B	1.644844	2.940832	0.508943	
B	3.285618	2.944500	0.562538	
B	4.901607	2.874855	0.742995	
B	6.525810	2.893146	1.098445	
B	8.010623	2.785903	1.607545	
B	-1.641117	2.939883	0.506975	
B	-3.273325	2.950084	0.589596	
B	-4.901604	2.896544	0.775436	
B	-6.548954	2.913562	1.044754	
B	-8.042070	2.752819	1.540297	
B	-0.003210	-2.913853	0.382270	
B	1.641328	-2.941080	0.409485	
B	3.276886	-2.946428	0.531085	
B	4.893496	-2.889849	0.761898	
B	6.499992	-2.890324	1.183861	
B	7.998897	-2.781651	1.656991	
B	-1.641083	-2.951733	0.339144	
B	-3.277777	-2.951220	0.485633	
B	-4.900026	-2.912621	0.721460	
B	-6.489819	-2.910643	1.190661	
B	-8.012039	-2.761850	1.608266	
B56				
#Energy = +2.60 eV (K)				
B	-3.198906	0.872858	0.307691	
B	2.419624	-0.779672	1.879181	
B	-2.032486	-3.239532	-1.144809	
B	1.089824	-2.295482	-1.919069	
B	0.408524	-2.859542	1.218911	
B	-3.383576	-0.714272	0.894181	
B	-1.179956	3.401138	-0.949719	
B	-0.247576	2.943798	-2.161419	
B	2.324864	-2.110402	-0.797749	
B	3.719094	0.303208	1.214011	
B	1.887824	-1.998872	0.836871	
B	-2.747836	-1.986432	-0.122659	
B	-1.543546	1.949658	-1.829249	
B	-0.242876	-1.880952	-2.976769	
B	1.139074	-1.731272	2.294131	



B	2.849264	0.754178	2.465091
B	2.981004	1.917108	1.224731
B	-2.709536	-1.716802	-1.793959
B	-2.253766	2.056878	1.348361
B	1.210634	2.237518	-2.385599
B	-0.219596	-2.589792	2.748271
B	-1.322456	-3.085972	1.627151
B	-0.262156	-0.175312	-3.299049
B	-1.771346	-1.037462	-3.074269
B	-3.021906	-0.201572	-2.418219
B	-0.379946	-2.969972	-1.599219
B	2.910544	3.085238	0.057711
B	-2.751776	0.534848	1.860741
B	1.874704	2.046608	2.573121
B	-2.364086	-3.482402	0.451301
B	3.101084	-1.033132	0.236851
B	1.204424	-1.069782	-3.191519
B	2.627474	1.288408	-2.252299
B	-0.266226	-1.024692	3.267401
B	-1.417866	1.335978	2.644531
B	-1.508786	3.343618	0.599011
B	-0.274016	1.455048	-2.901059
B	-2.932706	1.092468	-1.392909
B	0.812534	-2.937622	-0.408859
B	-0.870816	2.835558	2.022761
B	1.211874	0.573568	-2.800829
B	2.555894	2.668408	-1.452119
B	-1.661066	-2.725952	-2.678689
B	3.554624	1.637818	-0.536089
B	-2.419856	2.303648	-0.421909
B	-1.743426	-1.856872	2.785191
B	-2.866076	-2.238272	1.497871
B	-3.323376	-0.517202	-0.794519
B	0.198394	1.941608	3.140421
B	3.470594	-0.970942	-1.395909
B	-0.414446	0.528468	3.675751
B	2.036904	3.310738	1.408261
B	2.638524	-0.323982	-2.710829
B	-1.831456	-0.201842	3.124121
B	4.188804	0.098158	-0.346949
B	0.747314	3.239468	2.352641