

## Designing boron based stuffed fullerene clusters

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### Supplementary material

**S.1:** Energies (with ZPE correction) and relative energies of CBN clusters formed from each of the eight pentagonal pyramid isomers calculated at B3LYP/6-31G\* level. From isomer I five B<sub>84</sub> based clusters are generated 1a-1e, out of these four are having closed B<sub>84</sub> based structure, the remaining one is an open structure where bonds are broken. Similarly from II-2a-2f (6 closed B<sub>84</sub> based structure), from III-3a-3e (0 closed B<sub>84</sub> based structure), from IV-4a-4g (6 closed B<sub>84</sub> based structure), from V-5a-5e (0 closed B<sub>84</sub> based structure), from VI-6a-6c (3 closed B<sub>84</sub> based structure), from VI-7a-7d (0 closed B<sub>84</sub> based structure), from VII-8a-8c (0 closed B<sub>84</sub> based structure). Only clusters which maintained a closed B<sub>84</sub> based structure are taken for discussion even though they are higher in relative energies. A closed B<sub>84</sub> based structure will have a B<sub>12</sub>@B<sub>12</sub>@B<sub>60</sub> structure without any bonds broken. (See Fig.1,c and Fig.2,a in text)

S.No		Energy in a.u (E+ZPE)	Relative energy in kcal/mol
1	1a	-2789.413491	0.0
2	1b	-2788.964934	281.5 (4 closed str)
3	1c	-2789.040433	234.1
4	1d	-2789.100198	196.6
5	1e	-2788.124916	808.6
6	2a	-2789.158767	171.5
7	2b	-2789.404572	17.3
8	2c	-2789.432147	0.0 (6 closed str)
9	2d	-2789.321366	69.5
10	2e	-2789.309565	76.9
11	2f	-2789.276547	97.6
12	3a	-2789.690762	80.7
13	3b	-2630.924184	99706.7 (0 closed str)
14	3c	-2789.636004	115.1
15	3d	-2789.819461	0.0
16	3e	-2631.278209	99283.9
17	4a	-2789.598049	317.8
18	4b	-2789.927173	111.3
19	4c	-2790.100976	2.22 (6 closed str)
20	4d	-2790.096527	5.0
21	4e	-2790.104518	0.0
22	4f	-2789.960456	90.4
23	4g	-2790.029952	46.8
24	5a	-2790.459241	0.0
25	5b	-2789.937607	327.3

26	5c	-2789.738183	452.5 (0 closed str)
27	5d	-2789.972996	305.1
28	5e	-2789.514819	592.6
29	6a	-2789.802587	165.7
30	6b	-2790.066636	0.00 (3 closed str)
31	6c	-2790.065525	0.7
32	7a	-2,790.336525/	0.0
33	7b	-2789.882063	285.2 (0 closed str)
34	7c	-2789.617106	451.4
35	7d	-2790.190224	91.8
36	8a	-2790.851737	0.00
37	8b	-2790.036969	511.3 (0 closed str)
38	8c	-2790.734577	73.5

**S.2:** Cartesian coordinates of standard geometries of  $C_2B_3NH_6$  pentagonal pyramid isomers done at B3LYP/6-31G\* level.

I)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

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6	-0.783565	-0.071005	0.792142
6	-0.496691	1.012598	-0.230509
5	1.027566	1.099278	0.071078
1	-1.788955	-0.577798	-1.009976
1	1.395038	2.048084	0.705339
1	-1.256125	1.771880	-0.395632
1	-1.708233	-0.078052	1.359605
1	-0.163373	-2.376424	0.388887
1	2.746578	-0.842908	-0.460494
5	1.660352	-0.456283	-0.146100
5	0.200138	-1.247064	0.224793
7	-0.854811	-0.367714	-0.672340

II)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.349546	-1.177713	-0.200162
6	0.407438	1.159689	-0.209306
5	-1.182111	-0.809108	-0.340859
1	0.251632	0.001366	1.806869
1	-2.014580	-1.573164	0.051711
1	-1.933000	1.660839	0.066302
1	0.756080	2.073978	0.275743
1	2.546253	-0.062162	-0.223700
1	0.654716	-2.104801	0.290042
7	-0.007511	0.003752	0.821859
5	1.371935	-0.034133	-0.437118
5	-1.139910	0.860406	-0.334657

III)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.606698	-1.038918	-0.218986
5	0.230895	1.435590	-0.160137
1	-0.146168	-0.311155	1.851685
1	0.390609	2.519398	0.318415
1	2.552350	0.218188	-0.030184
1	0.853764	-2.054373	0.075629
1	-1.436680	-1.515976	0.093014
1	-2.364446	0.865787	-0.037267
7	-0.829144	-0.776717	-0.261519
5	-1.216386	0.689541	-0.311864
5	1.400539	0.263699	-0.346469
6	0.039858	0.000751	0.827601

IV)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.087559	-1.264820	-0.197995
5	0.770502	1.152732	-0.279475
1	-0.187409	0.053196	1.860397
1	1.105077	2.245009	0.057706
1	2.433712	-0.750834	0.073178
1	0.117865	-2.269628	0.219724
1	-2.359378	-0.807927	-0.079746
1	-1.366246	1.594155	0.185080
5	1.369721	-0.361517	-0.303020
5	-1.229057	-0.527968	-0.317730
7	-0.749088	0.886698	-0.211716
6	0.069802	0.000305	0.809129

V)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.032181	0.002848	0.976120
6	-1.198132	-0.337595	-0.251259
6	-0.046601	-1.166599	-0.248319
5	-0.836485	1.162441	-0.192667
1	0.149788	-0.304632	2.102467
1	-1.639215	2.006398	0.060763
1	1.735212	1.856728	-0.037588
1	1.986772	-0.758701	-0.006063
1	0.057472	-2.233901	-0.110929
1	-2.153539	-0.819838	-0.059905
5	0.800975	1.147380	-0.242978
7	1.095766	-0.326320	-0.236237

VI)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.064680	-0.000717	0.955996
6	-0.983912	-0.769226	-0.225600
1	0.031407	-0.010382	2.132648
1	-1.949629	1.236712	-0.002785
1	0.805913	2.370651	-0.145477
1	2.159683	0.068257	0.120488
1	0.950922	-2.315666	-0.144136
1	-1.870473	-1.352628	-0.002777
6	-1.029918	0.706881	-0.224572
5	0.358742	1.280360	-0.289796
7	1.185205	0.036510	-0.160800
5	0.437684	-1.255331	-0.292464

VII)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	0.000027	-0.030143	0.970870
1	0.000252	-0.445927	2.078623
1	-2.090366	-0.875735	-0.066272
1	-1.661402	1.993870	0.045709
1	1.659033	1.995903	0.045579
1	2.091471	-0.873263	-0.066392
1	0.001271	-2.089522	-0.050545
6	-1.188394	-0.295250	-0.232913
5	-0.837640	1.168462	-0.203152
5	0.835981	1.169692	-0.202947
6	1.188864	-0.293722	-0.232964
7	0.000725	-1.101649	-0.287898

VIII)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.040159	-0.034247	0.961478
1	0.174373	-0.183029	2.114622
1	-0.527843	-2.211903	-0.035727
1	-2.544173	-0.029366	-0.166658
1	-0.731505	2.227371	0.167798
1	2.088119	1.377418	-0.191075
1	1.708762	-1.272847	0.011761
6	-0.418970	-1.150184	-0.215715
5	-1.363914	0.026266	-0.314711
7	0.949029	-0.645986	-0.232684
6	-0.410327	1.231338	-0.119043
5	1.037042	0.833447	-0.299444

**S.3:** Cartesian coordinates of optimized structures of B<sub>84</sub> based CBN clusters with closed and lower energy structures taken from the 38 clusters made from each of the eight pentagonal pyramid isomers computed at B3LYP/6-31G\* level.

1)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.104406	1.357747	0.828121
5	1.328831	0.811045	0.192373
5	0.104406	-1.357747	-0.828121
5	-1.328831	-0.811045	-0.192373
5	1.305591	-0.844940	0.196421
5	-1.305591	0.844940	-0.196421

5	-0.143099	-1.349746	0.834109
5	1.025370	-0.017666	-1.222444
5	-1.025370	0.017666	1.222444
5	0.143099	1.349746	-0.834109
5	3.399756	-1.043424	-2.089656
5	-3.133828	1.800097	-1.978405
5	0.042875	4.071162	0.711374
5	-2.318343	3.199617	-1.387252
5	-2.629976	3.151667	0.302049
5	0.149744	-2.768240	3.254125
5	-2.210603	1.588640	3.186769
5	2.318343	-3.199617	1.387252
5	3.133828	-1.800097	1.978405
5	0.468549	2.860566	3.128063
5	-1.257184	-3.577049	-1.790750
5	2.629976	-3.151667	-0.302049
5	-3.399756	1.043424	2.089656
5	-0.149744	2.768240	-3.254125
5	-1.594816	0.175511	3.973551
5	-3.327213	-1.502028	-1.903795
5	-1.798642	-3.416471	1.441471
5	-4.079595	-0.588863	-0.669573
5	-0.042875	-4.071162	-0.711374
5	-3.780278	-1.461297	0.766488
5	1.542704	2.583778	-2.917033
5	3.780278	1.461297	-0.766488
5	-0.468549	-2.860566	-3.128063
5	4.079595	0.588863	0.669573
5	3.327213	1.502028	1.903795
5	1.594816	-0.175511	-3.973551
5	1.059029	-1.367398	3.894317
5	2.210603	-1.588640	-3.186769
5	0.158034	0.031816	4.317617
5	1.123976	1.375972	3.858215
5	-1.542704	-2.583778	2.917033
5	-1.059029	1.367398	-3.894317
5	1.257184	3.577049	1.790750
5	1.798642	3.416471	-1.441471
5	-1.123976	-1.375972	-3.858215
5	-0.158034	-0.031816	-4.317617
6	-0.604920	0.004461	-1.421627
6	0.604920	-0.004461	1.421627
6	2.409889	-0.819776	3.139077
6	2.451770	0.743743	3.118998
6	-2.451770	-0.743743	-3.118998
6	-2.409889	0.819776	-3.139077
6	-2.683654	-2.836864	-1.202449
6	-2.931392	-2.798812	0.330346
6	2.931392	2.798812	-0.330346
6	2.683654	2.836864	1.202449
6	-3.877682	1.087983	-0.707360
6	-3.582005	1.851352	0.608810

6	3.877682	-1.087983	0.707360
6	3.582005	-1.851352	-0.608810
6	0.758396	-3.561080	1.950858
6	-0.342921	-3.958066	0.935502
6	0.342921	3.958066	-0.935502
6	-0.758396	3.561080	-1.950858
6	1.135691	-2.861051	-2.724888
6	1.372165	-3.575330	-1.361483
6	-1.372165	3.575330	1.361483
6	-1.135691	2.861051	2.724888
6	-3.393525	-0.590801	2.165100
6	-2.347126	-1.086378	3.205804
6	2.347126	1.086378	-3.205804
6	3.393525	0.590801	-2.165100
7	1.935540	-0.112597	-2.263361
7	0.124232	-2.556317	-1.525703
7	-2.543259	-1.438203	-0.398642
7	-2.415366	1.631228	-0.441190
7	0.332964	2.490222	-1.600040
7	-0.124232	2.556317	1.525703
7	2.543259	1.438203	0.398642
7	2.415366	-1.631228	0.441190
7	-0.332964	-2.490222	1.600040
7	-1.935540	0.112597	2.263361
7	1.112455	-0.006167	2.693312
7	-1.112455	0.006167	-2.693312

2)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-1.066014	-0.833133	-0.835918
5	-0.514399	0.645432	-1.361295
5	1.066014	0.833133	0.835918
5	0.514399	-0.645432	1.361295
6	-0.172932	1.502791	-0.002916
5	-1.496892	0.545695	-0.004464
6	0.172932	-1.502791	0.002916
5	1.496892	-0.545695	0.004464
5	-0.519298	0.646649	1.358856
5	1.071352	0.832038	-0.833390
5	-1.071352	-0.832038	0.833390
5	0.519298	-0.646649	-1.358856
6	1.968118	3.175544	-1.729325
6	0.791427	-3.761939	1.297579
5	1.815354	-3.733845	0.034394
6	-2.610131	-1.004492	3.003661
5	-1.565109	-2.327933	-3.066596
6	0.826355	-3.742181	-1.272637
6	1.947074	3.180237	1.744064
6	-2.517098	1.845178	2.683234

6	-0.826355	3.742181	1.272637
5	-1.815354	3.733845	-0.034394
6	-3.540744	-1.164719	-1.694725
5	-1.577305	-2.251976	3.022425
6	-0.791427	3.761939	-1.297579
6	-1.968118	-3.175544	1.729325
6	2.517098	-1.845178	-2.683234
5	1.565109	2.327933	3.066596
6	3.540744	1.164719	1.694725
6	-1.947074	-3.180237	-1.744064
6	-2.098959	0.559462	-3.495101
5	-3.277480	2.703608	-0.040888
6	-4.008069	0.244381	0.828816
5	1.577305	2.251976	-3.022425
6	-3.535650	1.691491	-1.291892
5	3.277480	-2.703608	0.040888
6	3.535650	-1.691491	1.291892
6	2.610131	1.004492	-3.003661
7	-0.300175	2.856768	-0.006910
7	0.300175	-2.856768	0.006910
7	-1.963565	-1.580940	-1.583794
7	0.961659	-1.220811	-2.539119
7	2.777178	-1.078114	-0.008459
7	0.985649	-1.256235	2.512269
7	-2.004715	-1.582976	1.533756
7	1.963565	1.580940	1.583794
7	2.004715	1.582976	-1.533756
7	-0.985649	1.256235	-2.512269
7	-2.777178	1.078114	0.008459
7	-0.961659	1.220811	2.539119
5	2.577412	-1.863811	2.674652
5	3.990604	-0.205443	0.793702
5	-0.743454	-3.934535	-0.859113
5	-0.756297	-3.940297	0.860981
5	1.204790	-2.902636	2.676148
5	0.590308	-0.690908	4.101558
6	2.098959	-0.559462	3.495101
6	0.042910	-2.119316	3.515588
5	-3.597852	-1.134565	1.713862
5	-3.247488	-2.603901	0.894428
5	-2.629925	-0.976535	-3.038443
5	-3.206278	-2.564614	-0.909803
5	1.238262	-2.844160	-2.639980
5	0.517651	-0.728141	-4.157576
5	2.107318	-0.519886	-3.530569
6	0.051480	-2.150038	-3.525797
6	4.008069	-0.244381	-0.828816
5	3.538272	-1.714625	-1.341544
5	0.756297	3.940297	-0.860981
5	0.743454	3.934535	0.859113
5	-3.990604	0.205443	-0.793702
5	-3.538272	1.714625	1.341544



5	-0.590308	0.690908	-4.101558
5	-1.204790	2.902636	-2.676148
5	-2.577412	1.863811	-2.674652
6	-0.042910	2.119316	-3.515588
5	3.597852	1.134565	-1.713862
5	3.247488	2.603901	-0.894428
5	2.629925	0.976535	3.038443
5	3.206278	2.564614	0.909803
5	-2.107318	0.519886	3.530569
5	-0.517651	0.728141	4.157576
5	-1.238262	2.844160	2.639980
6	-0.051480	2.150038	3.525797

3)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.253729	1.379271	0.838462
5	1.281484	0.986639	0.173575
5	0.253729	-1.379271	-0.838462
5	-1.281484	-0.986639	-0.173575
5	1.456365	-0.736832	0.188434
5	-1.456365	0.736832	-0.188434
5	-0.013118	-1.418887	0.869547
5	1.064322	0.075724	-1.262790
5	-1.064322	-0.075724	1.262790
5	0.013118	1.418887	-0.869547
5	3.304742	-1.377167	-1.912735
5	-3.482271	1.735566	-2.041706
5	0.281673	3.980879	0.440883
5	-2.543252	3.055678	-1.557029
5	-2.350538	3.315071	0.162988
5	0.123485	-3.203355	3.342506
5	-2.254004	1.519774	3.272189
5	2.543252	-3.055678	1.557029
5	3.482271	-1.735566	2.041706
5	0.377402	2.796732	3.392789
5	-1.140272	-3.454691	-2.009051
5	2.350538	-3.315071	-0.162988
5	-3.304742	1.377167	1.912735
5	-0.123485	3.203355	-3.342506
5	-1.997306	0.145547	4.141338
5	-3.301258	-1.560522	-2.129677
5	-2.055103	-3.129821	1.577044
5	-4.111976	-0.795542	-0.845623
5	-0.281673	-3.980879	-0.440883
5	-3.800123	-1.155867	0.883715
5	1.378078	2.599316	-3.068079
5	3.800123	1.155867	-0.883715
5	-0.377402	-2.796732	-3.392789
5	4.111976	0.795542	0.845623
5	3.301258	1.560522	2.129677

5	1.997306	-0.145547	-4.141338
5	1.301799	-1.583505	3.587997
5	2.254004	-1.519774	-3.272189
5	0.166575	-0.414960	4.035601
5	0.965472	1.078638	3.892343
5	-1.378078	-2.599316	3.068079
5	-1.301799	1.583505	-3.587997
5	1.140272	3.454691	2.009051
5	2.055103	3.129821	-1.577044
5	-0.965472	-1.078638	-3.892343
5	-0.166575	0.414960	-4.035601
6	-0.610315	-0.032985	-1.359712
6	0.610315	0.032985	1.359712
6	2.570839	-0.862879	3.140178
6	-2.570839	0.862879	-3.140178
6	-2.385922	-2.672701	-1.700097
6	2.385922	2.672701	1.700097
6	-3.934843	0.662373	-1.129963
6	3.934843	-0.662373	1.129963
6	1.284562	-3.035578	2.517065
6	-1.284562	3.035578	-2.517065
6	0.997772	-2.405229	-3.137299
6	-0.997772	2.405229	3.137299
6	-1.484027	-1.093084	3.622272
6	1.484027	1.093084	-3.622272
6	-1.144168	0.078500	-2.691918
6	0.407600	-2.634001	-1.699163
6	-2.487179	-1.870712	-0.476158
6	-2.806647	1.391974	-0.470292
6	0.080779	2.707453	-1.711883
6	2.063630	0.053818	-2.426052
6	-0.407600	2.634001	1.699163
6	-2.063630	-0.053818	2.426052
6	-0.080779	-2.707453	1.711883
6	2.806647	-1.391974	0.470292
6	2.487179	1.870712	0.476158
6	1.144168	-0.078500	2.691918
7	-2.411604	-0.613505	-3.203092
7	2.411604	0.613505	3.203092
7	0.822112	3.707203	-0.880313
7	-0.822112	-3.707203	0.880313
7	3.451820	0.118107	-1.843545
7	-3.451820	-0.118107	1.843545
7	1.094485	-3.692449	-0.840026
7	-1.094485	3.692449	0.840026
7	-3.058486	-2.417921	0.802302
7	3.058486	2.417921	-0.802302
7	-3.187897	2.207409	0.720698
7	3.187897	-2.207409	-0.720698

4)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.188154	1.537508	-0.173271
5	1.136730	0.738776	-0.738606
5	0.188154	-1.537508	0.173271
5	-1.136730	-0.738776	0.738606
5	1.460726	-0.520819	0.260765
5	-1.460726	0.520819	-0.260765
5	0.309515	-0.502591	1.440562
5	0.700992	-0.771947	-1.178429
5	-0.700992	0.771947	1.178429
5	-0.309515	0.502591	-1.440562
5	-3.965132	0.091668	-1.406000
5	-3.263370	1.515936	-2.006420
5	1.591343	-0.074045	3.775155
5	3.263370	-1.515936	2.006420
5	3.965132	-0.091668	1.406000
5	-1.591343	0.074045	-3.775155
5	-3.208146	-2.500373	0.629813
5	-3.785491	-0.999127	1.197042
5	0.028196	0.227410	-4.176830
5	3.785491	0.999127	-1.197042
5	3.208146	2.500373	-0.629813
5	0.943815	2.606489	2.879593
5	1.498512	3.421871	1.499414
5	-0.028196	-0.227410	4.176830
5	0.738734	3.799108	-1.207163
5	-1.498512	-3.421871	-1.499414
6	-0.864873	-0.868397	-0.841662
6	0.864873	0.868397	0.841662
6	2.832542	2.668060	1.022496
6	-2.832542	-2.668060	-1.022496
6	-2.100146	-3.014787	1.733711
6	2.100146	3.014787	-1.733711
6	-4.084823	0.334821	0.215340
6	4.084823	-0.334821	-0.215340
6	2.074326	-1.497122	3.177990
6	-2.074326	1.497122	-3.177990
6	1.366625	-1.437827	-2.278622
6	0.403637	-2.952176	0.354510
6	-2.198516	-1.459238	1.378862
6	-2.818156	0.916800	-0.543602
6	-0.625977	0.912599	-2.783705
6	-0.403637	2.952176	-0.354510
6	2.198516	1.459238	-1.378862
6	2.818156	-0.916800	0.543602
6	0.625977	-0.912599	2.783705
6	-1.366625	1.437827	2.278622
6	1.651121	1.749745	1.600313
6	-1.651121	-1.749745	-1.600313
5	-3.271087	-1.465684	-1.968576

5	-0.943815	-2.606489	-2.879593
7	-2.016948	-1.423035	-3.062277
7	2.016948	1.423035	3.062277
5	3.271087	1.465684	1.968576
5	2.611637	-0.761070	-3.088105
5	1.877690	-3.591034	0.677895
5	-1.877690	3.591034	-0.677895
5	-1.881268	-1.975640	2.917429
7	-2.920535	-0.801813	2.600140
7	2.920535	0.801813	-2.600140
5	1.881268	1.975640	-2.917429
5	-3.584740	1.778960	0.661944
7	-3.094516	2.467072	-0.708199
7	3.094516	-2.467072	0.708199
5	3.584740	-1.778960	-0.661944
5	-0.870125	2.523077	-3.048806
7	0.422383	1.702249	-3.617248
7	-0.422383	-1.702249	3.617248
5	0.870125	-2.523077	3.048806
7	0.443624	3.994875	0.373010
6	-0.714015	3.577526	-1.805822
5	-1.125995	3.954677	0.784545
5	-2.611637	0.761070	3.088105
7	-0.443624	-3.994875	-0.373010
6	0.714015	-3.577526	1.805822
5	1.125995	-3.954677	-0.784545
5	-0.738734	-3.799108	1.207163
7	-0.621557	2.375717	3.228873
5	-1.658657	3.099317	2.227250
6	-2.844824	2.036445	2.117977
5	-1.182068	1.013682	3.900430
5	1.182068	-1.013682	-3.900430
5	1.658657	-3.099317	-2.227250
7	0.621557	-2.375717	-3.228873
6	2.844824	-2.036445	-2.117977

5)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.141612	1.241528	0.871599
5	1.241580	0.772512	0.178493
5	0.141612	-1.241528	-0.871599
5	-1.241580	-0.772512	-0.178493
5	1.287179	-0.807335	0.140009
5	-1.287179	0.807335	-0.140009
5	-0.088405	-1.318139	0.836593
5	1.066611	0.073204	-1.364549
5	-1.066611	-0.073204	1.364549
5	0.088405	1.318139	-0.836593

5	-3.282472	1.805230	-2.021335
5	0.910945	-2.751693	3.219694
5	3.282472	-1.805230	2.021335
5	0.392834	2.815363	3.068052
5	-0.910945	2.751693	-3.219694
5	-1.215607	-0.226750	3.934462
5	-3.296254	-1.428186	-1.987432
5	-0.392834	-2.815363	-3.068052
5	3.296254	1.428186	1.987432
5	1.215607	0.226750	-3.934462
5	0.440597	-0.144969	4.284400
5	1.251247	1.295036	3.830900
5	-1.251247	-1.295036	-3.830900
5	-0.440597	0.144969	-4.284400
6	-0.592405	0.028612	-1.394858
6	0.592405	-0.028612	1.394858
6	2.583365	-0.937398	3.166917
6	-2.947984	-2.757477	0.257637
6	2.947984	2.757477	-0.257637
6	-3.579725	1.949066	0.533925
6	3.579725	-1.949066	-0.533925
6	-0.466029	-3.846766	0.851558
6	0.466029	3.846766	-0.851558
6	1.400057	-3.649596	-1.142881
6	-1.400057	3.649596	1.142881
6	-3.234414	-0.311535	1.745850
6	3.234414	0.311535	-1.745850
5	0.154025	-2.587642	-1.497599
5	-2.524438	-1.425019	-0.499518
5	-2.411573	1.700961	-0.564305
5	0.256551	2.482984	-1.842726
5	2.041437	-1.070777	-3.707621
5	-0.154025	2.587642	1.497599
5	2.524438	1.425019	0.499518
5	2.411573	-1.700961	0.564305
5	-0.256551	-2.482984	1.842726
5	-2.041437	1.070777	3.707621
5	1.224073	-0.066393	2.748639
5	-1.224073	0.066393	-2.748639
7	-1.081888	-3.518785	-1.752067
5	1.391538	-3.025466	-2.573434
6	-0.042745	-3.885388	-0.611803
6	-3.647837	-1.270880	0.583495
7	-3.915335	-0.633375	-0.745655
5	-2.617717	-2.897248	-1.293919
7	-2.600805	-0.619707	-3.126081
6	-2.583365	0.937398	-3.166917
6	-1.361800	1.367085	-3.823095
7	2.600805	0.619707	3.126081
6	1.361800	-1.367085	3.823095
7	1.081888	3.518785	1.752067
5	-1.391538	3.025466	2.573434

6	0.042745	3.885388	0.611803
7	3.915335	0.633375	0.745655
5	2.617717	2.897248	1.293919
6	3.647837	1.270880	-0.583495
7	-2.395703	3.081378	-1.294805
5	-3.980543	1.076959	-0.747316
6	-2.590987	3.097400	0.198968
6	2.590987	-3.097400	-0.198968
5	3.980543	-1.076959	0.747316
7	2.395703	-3.081378	1.294805
7	1.684573	2.536526	-2.411603
5	-0.918368	3.692916	-1.923049
6	1.827335	3.215570	-1.240198
6	-1.827335	-3.215570	1.240198
5	0.918368	-3.692916	1.923049
7	-1.684573	-2.536526	2.411603
7	2.565839	-1.880674	-2.761087
5	2.114249	1.009698	-2.680148
6	3.313578	-1.156091	-1.750959
6	-3.313578	1.156091	1.750959
5	-2.114249	-1.009698	2.680148
7	-2.565839	1.880674	2.761087

6)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.274504	1.362108	0.567006
5	1.185198	0.734767	0.634414
5	0.274504	-1.362108	-0.567006
5	-1.185198	-0.734767	-0.634414
5	1.000270	-0.842976	0.753070
5	-1.000270	0.842976	-0.753070
5	-0.553583	-1.176401	0.770519
5	1.338033	-0.194944	-0.648119
5	-1.338033	0.194944	0.648119
5	0.553583	1.176401	-0.770519
5	3.813416	-1.220532	-0.466208
5	-2.353254	3.164356	-1.079012
5	-3.813416	1.220532	0.466208
5	-2.405507	-3.165329	0.931215
5	-3.847856	-1.381182	-0.563225
5	3.847856	1.381182	0.563225
5	-0.574545	-0.970923	3.874395
5	-0.297582	1.754491	3.574288
5	0.574545	0.970923	-3.874395
5	2.405507	3.165329	-0.931215
5	0.297582	-1.754491	-3.574288
6	0.004469	-0.120123	-1.439712

6	-0.004469	0.120123	1.439712
6	0.970633	-0.548638	3.841902
6	1.127514	1.048969	3.718551
6	-1.127514	-1.048969	-3.718551
6	-0.970633	0.548638	-3.841902
5	-1.089349	-2.301514	1.549754
5	1.966925	-1.622943	1.538915
5	2.307540	1.508731	1.220279
5	-2.660902	0.344937	1.257339
5	-0.551178	2.712005	1.067115
5	-1.966925	1.622943	-1.538915
5	-2.307540	-1.508731	-1.220279
5	0.551178	-2.712005	-1.067115
5	2.660902	-0.344937	-1.257339
5	1.089349	2.301514	-1.549754
5	-0.013515	-0.260848	-2.861558
5	0.013515	0.260848	2.861558
7	-1.326851	0.501169	3.673536
7	1.326851	-0.501169	-3.673536
7	3.434553	-1.847149	0.985549
5	3.253600	-0.812392	2.245372
5	2.353254	-3.164356	1.079012
6	1.595287	-2.880471	2.452842
6	2.081919	-1.489536	3.122145
6	-2.081919	1.489536	-3.122145
6	-1.595287	2.880471	-2.452842
7	-3.434553	1.847149	-0.985549
5	-3.253600	0.812392	-2.245372
5	-2.033117	3.002516	1.735333
5	2.033117	-3.002516	-1.735333
7	-0.810906	-3.773659	1.070688
5	-0.054840	-3.251179	2.470567
6	-2.530400	-2.247268	2.242056
6	-1.195569	-2.330607	3.139748
6	1.195569	2.330607	-3.139748
6	2.530400	2.247268	-2.242056
5	0.054840	3.251179	-2.470567
7	0.810906	3.773659	-1.070688
5	-2.718785	0.491457	2.895447
7	-3.076838	1.756747	1.860310
6	-3.330857	-0.795477	2.155400
6	-4.004462	-0.351515	0.749986
5	2.396474	1.721476	2.873596
7	-0.638497	3.004848	2.599722
7	3.436857	0.756484	2.045193
6	3.045794	2.757719	0.545218
6	2.205518	2.965254	1.878178
6	-0.031531	4.009309	0.310263
5	0.702730	3.643836	1.688126
6	-1.609986	3.691267	0.338893
6	4.004462	0.351515	-0.749986
5	2.718785	-0.491457	-2.895447

6	3.330857	0.795477	-2.155400
7	3.076838	-1.756747	-1.860310
7	-3.436857	-0.756484	-2.045193
5	-2.396474	-1.721476	-2.873596
6	-2.205518	-2.965254	-1.878178
6	-3.045794	-2.757719	-0.545218
6	1.609986	-3.691267	-0.338893
6	0.031531	-4.009309	-0.310263
7	0.638497	-3.004848	-2.599722
5	-0.702730	-3.643836	-1.688126

7)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.739482	-1.454425	-0.255519
5	-0.743745	-0.302496	-1.648662
5	0.711646	1.430087	-0.100770
5	0.836322	0.313014	1.244860
5	-0.845805	1.247244	-0.852522
5	0.836245	-1.352928	0.593899
5	-0.657964	1.100348	0.890482
5	0.739427	0.493597	-1.572961
5	-0.646131	-0.587003	1.333197
5	0.660859	-1.186725	-1.118585
5	-1.049720	-3.380540	-2.240534
5	0.333831	-4.233000	0.099231
5	-0.062576	1.326511	3.755817
5	1.184453	3.480976	2.016521
5	1.648613	-1.201457	3.444507
5	-1.655569	1.569683	-3.029146
5	4.030346	-0.514998	-1.737482
5	0.501606	-1.962965	-3.630653
5	3.956773	1.703834	-0.351221
6	1.533238	-0.029457	-0.222091
6	-1.542039	-0.017873	-0.005376
6	4.242996	0.493961	0.617550
6	4.390916	-0.775788	-0.202111
5	-1.031378	2.070091	2.284294
5	-1.989447	2.543528	-1.640260
5	-1.723031	-1.248694	-3.295069
5	-0.203092	-1.134739	3.571768
5	-1.247947	-3.017808	-0.495242
5	1.913623	-2.795331	0.926536
5	1.392997	1.033407	2.656576
5	1.376241	2.894777	0.236701
5	0.181498	1.020404	-3.564423
5	1.343719	-2.732048	-1.385694
5	3.036786	0.141551	-0.456064
5	-3.048994	-0.026873	0.292429



7	-3.671593	-1.003001	1.718295
7	3.661066	1.030563	-1.677122
5	-0.992121	3.919610	0.083591
6	-3.699114	2.346439	-0.002404
6	3.898794	-2.012384	0.337165
6	-3.686887	-0.263012	-1.946757
6	3.596099	0.422284	1.942866
6	-3.261103	-2.665797	-0.080526
6	3.184510	2.955870	0.142096
6	-2.986479	1.315368	2.601707
6	3.116750	-1.485557	-2.512356
6	-3.835805	0.511605	1.760607
6	-3.981565	-1.522994	0.383995
5	-4.422324	1.038284	0.442551
5	-4.456470	-0.330706	-0.594536
5	-1.751430	0.678580	3.182844
6	0.399824	2.489836	2.904805
7	-2.505561	2.594902	2.203618
5	-1.778982	-3.117901	1.981912
5	-2.768993	-2.555524	-1.541908
6	0.075646	-3.865956	-1.260202
7	-2.230429	-3.406686	0.612571
7	-2.973988	-1.394617	-2.396695
7	-3.428575	2.354122	-1.334188
5	-3.278257	1.257636	-2.260691
6	-1.133357	0.123179	-3.363886
6	-0.909874	3.638636	-1.480126
5	-2.624595	3.120814	0.880159
7	3.253134	-2.107827	1.541956
5	3.062018	-2.970892	-0.512211
6	0.730970	-3.766270	1.450531
7	2.887868	1.496868	2.353275
5	3.046596	-1.021445	2.451897
6	0.804149	0.017639	3.950455
7	2.230922	3.713830	-0.682740
5	2.730407	2.794016	1.585590
6	0.248221	4.008860	0.964175
5	1.702268	3.106784	-1.922922
7	2.761207	-2.703639	-1.857770
5	1.884024	-0.962849	-3.273913
6	-0.819232	-2.522647	-3.460574
7	0.496491	-2.348150	3.361683
6	-0.120750	-3.267197	2.426350
6	-1.470822	-0.767448	2.851039
5	-2.556207	-1.712457	2.442668
5	2.473549	1.617429	-2.438193
6	0.134445	3.304447	-2.369084
6	1.557939	0.582161	-3.091962
7	-0.388077	2.348004	-3.329964

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.032327	1.262830	1.080742
5	1.372296	0.942392	0.082033
5	0.032327	-1.262830	-1.080742
5	-1.372296	-0.942392	-0.082033
5	1.460807	-0.788734	-0.141942
5	-1.460807	0.788734	0.141942
5	0.117350	-1.500873	0.624160
5	0.864453	0.311728	-1.414708
5	-0.864453	-0.311728	1.414708
5	-0.117350	1.500873	-0.624160
5	3.185345	-1.228345	-2.254437
5	0.355066	3.806121	0.631265
5	-1.747583	3.646055	-0.749652
5	-3.185345	1.228345	2.254437
5	-1.888951	-3.303212	1.624910
5	-0.355066	-3.806121	-0.631265
5	-4.145902	-0.084123	0.273588
5	4.145902	0.084123	-0.273588
5	1.170792	-1.321686	3.951484
5	-1.170792	1.321686	-3.951484
5	1.888951	3.303212	-1.624910
6	-0.818157	0.118015	-1.281050
6	0.818157	-0.118015	1.281050
6	2.597016	-0.843495	3.464451
6	-2.597016	0.843495	-3.464451
5	-0.021958	-2.955872	1.427683
5	2.953500	-1.572116	-0.154909
5	2.607635	2.146793	0.074895
5	-3.006574	-1.282862	2.038350
5	-1.933522	3.108053	1.632542
5	-2.953500	1.572116	0.154909
5	-2.607635	-2.146793	-0.074895
5	1.933522	-3.108053	-1.632542
5	3.006574	1.282862	-2.038350
5	0.021958	2.955872	-1.427683
5	-1.405489	0.083288	-2.691445
5	1.405489	-0.083288	2.691445
7	0.344002	-0.020540	3.972897
7	-0.344002	0.020540	-3.972897
7	3.209695	-2.395106	-1.325360
5	1.747583	-3.646055	0.749652
6	2.618217	-3.012420	1.813461
6	-2.618217	3.012420	-1.813461
7	-3.209695	2.395106	1.325360
6	4.029440	0.631684	1.100556
7	3.091594	2.528180	-1.270044
7	-3.091594	-2.528180	1.270044
6	-4.029440	-0.631684	-1.100556

7	-1.206955	3.847205	0.587889
6	1.171551	3.126060	1.835096
6	-1.171551	-3.126060	-1.835096
7	1.206955	-3.847205	-0.587889
7	-3.766681	-0.049455	1.672690
6	-1.984261	1.321360	3.292498
6	1.984261	-1.321360	-3.292498
7	3.766681	0.049455	-1.672690
7	-0.928799	-3.912458	0.715605
6	-1.038928	-2.595850	2.800569
6	1.038928	2.595850	-2.800569
7	0.928799	3.912458	-0.715605
6	1.153341	1.199062	3.707499
5	2.648477	0.788594	3.500430
6	-1.153341	-1.199062	-3.707499
5	-2.648477	-0.788594	-3.500430
6	-1.647301	-1.189770	2.818625
5	-1.161503	0.026446	3.598831
5	0.367721	2.353141	2.913421
6	-1.210612	2.416654	2.877014
6	2.516145	2.698152	1.506513
5	3.365035	1.607100	2.216345
5	3.255115	-1.646615	2.293220
6	3.865863	-0.783112	1.044839
6	1.378230	-3.433914	2.273384
5	0.386554	-2.711687	3.328211
5	-0.386554	2.711687	-3.328211
6	-1.378230	3.433914	-2.273384
6	-3.865863	0.783112	-1.044839
5	-3.255115	1.646615	-2.293220
5	-3.365035	-1.607100	-2.216345
6	-2.516145	-2.698152	-1.506513
6	1.210612	-2.416654	-2.877014
5	-0.367721	-2.353141	-2.913421
5	1.161503	-0.026446	-3.598831
6	1.647301	1.189770	-2.818625

**S.4:** Global minimum structure and energy of  $C_{14}B_{58}N_{12}Li_{12}$  computed at B3LYP/6-31G\* level.

E=

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	1.105727	0.887288	-0.828956
5	1.555883	-0.082805	0.516926
5	-1.105767	-0.887387	0.828964
5	-1.555881	0.082876	-0.516838
6	0.218143	-0.113413	1.537283
5	0.593069	1.335839	0.745919

6	-0.218032	0.113345	-1.537178
5	-0.593068	-1.335765	-0.745812
5	-1.056569	0.833767	0.945224
5	0.510214	-1.463586	0.554162
5	-0.510502	1.463777	-0.553725
5	1.056616	-0.834119	-0.944634
6	1.026818	1.008788	3.832536
5	-0.564516	0.623427	4.093150
5	2.014106	-0.298867	3.658835
5	0.938059	-1.681797	3.674459
5	-0.672305	-1.133385	4.036789
5	0.564778	-0.623232	-4.092792
5	-2.014190	0.298769	-3.658950
5	0.672390	1.133546	-4.036993
5	-0.937938	1.681580	-3.674511
6	-1.026775	-1.008748	-3.832306
5	-2.045508	-1.901338	3.282014
5	-1.721542	-3.229402	2.221650
5	-2.743063	-3.002903	0.818290
5	-1.901484	1.587027	3.487598
5	-1.526381	3.013395	2.528111
5	-3.527123	1.752853	1.270835
5	2.752722	2.542756	1.976412
5	0.755971	4.072591	0.906808
5	0.148528	3.492486	2.442383
5	3.407756	-0.244382	2.635061
5	3.762525	1.171728	1.746566
5	4.082009	0.666037	0.124481
5	2.011742	-3.710672	0.171276
5	-0.075525	-3.751283	1.973677
5	0.396948	-4.263227	0.382100
5	2.045462	1.901525	-3.282193
5	1.721555	3.229394	-2.221614
5	2.743086	3.002787	-0.818353
5	1.901886	-1.587104	-3.487560
5	3.528293	-1.751970	-1.271248
5	1.525826	-3.013795	-2.529957
5	-0.148855	-3.492822	-2.442646
5	-0.755997	-4.072720	-0.907190
5	-2.753040	-2.542704	-1.976377
5	-3.407921	0.244678	-2.635163
5	-4.081872	-0.665843	-0.124423
5	-3.762664	-1.171494	-1.746721
5	-2.012136	3.711895	-0.171964
5	-0.396960	4.263301	-0.382469
5	0.075504	3.750912	-1.973861
7	-2.041842	-1.654393	1.595635
7	0.403298	-0.246949	2.921097
7	0.943132	-2.738377	1.039781
7	2.901891	-0.127634	1.017125
7	1.104763	2.464396	1.457490
7	-1.967384	1.514208	1.814777

7	-0.943130	2.738843	-1.039347
7	2.041718	1.654285	-1.595802
7	1.967191	-1.516970	-1.812451
7	-1.105034	-2.464404	-1.457120
7	-2.901746	0.127785	-1.017258
7	-0.403050	0.246776	-2.921002
5	1.385471	2.462939	3.087282
6	2.247607	3.428750	0.709510
6	4.012635	-0.970792	0.089519
5	3.595793	-1.588195	1.558319
5	2.534380	-2.947740	1.644462
6	1.228723	-2.962018	2.639669
6	-3.621066	-1.639175	1.111684
5	-3.285650	-0.924828	2.551996
5	-3.241343	0.805946	2.708132
6	-2.549004	3.051721	1.249042
6	-2.247728	-3.428735	-0.709674
5	-1.385651	-2.462843	-3.087162
6	-4.012219	0.970875	-0.089248
5	-3.595546	1.588303	-1.558206
5	-2.534316	2.948031	-1.644915
6	-1.228713	2.961773	-2.639860
6	3.621109	1.639166	-1.111761
5	3.285344	0.924866	-2.552117
5	3.241482	-0.806021	-2.708321
6	2.548446	-3.050277	-1.250038
3	2.066543	4.537407	2.678018
3	0.799194	-0.429323	5.495772
3	5.407538	-0.292061	1.665247
3	3.854200	3.076767	-2.772149
3	-1.762638	5.010679	-1.958772
3	-3.656564	2.914959	3.196025
3	1.763580	-5.010115	1.957843
3	-3.854077	-3.076926	2.772041
3	-0.798978	0.428800	-5.495659
3	-5.407639	0.292429	-1.664616
3	-2.066820	-4.536747	-2.678961
3	3.656538	-2.916193	-3.193650

**S.5:** Optimized geometry and energy of  $\text{CB}_4\text{LiNH}_6$  computed at B3LYP/6-31G\* level.

E=

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	0.003927	-1.253484	0.171356
5	-0.853270	1.183359	0.119634
1	0.000160	-0.198082	-1.850683
1	-1.513680	1.997059	-0.457754

1	-2.328179	-0.937883	-0.281261
1	0.006535	-2.240204	-0.293786
1	2.334199	-0.923276	-0.281676
1	1.501340	2.006010	-0.458207
5	0.845901	1.188455	0.119372
5	1.350542	-0.419588	0.172622
7	-0.000112	-0.027702	-0.845428
5	-1.347803	-0.427710	0.172864
3	-0.000002	0.129534	1.863588

**S.6:** Optimized structure and energy of CBN cluster with some borons replaced by Al atoms done at B3LYP/6-31G\* level.

E=

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-1.375019	-0.332417	0.706841
5	-0.735222	1.209446	0.737686
5	1.385362	0.349869	-0.696803
5	0.740119	-1.192509	-0.713205
5	0.937535	1.077193	0.719280
5	-0.929971	-1.060182	-0.696230
5	1.323871	-0.546816	0.681895
5	0.106559	1.427360	-0.660640
5	-0.101973	-1.415899	0.674593
5	-1.323745	0.566425	-0.670773
5	-1.264589	0.661713	-3.873117
5	1.349080	0.157775	-3.893823
6	-0.010530	0.028829	-1.429544
6	0.013681	-0.022293	1.452415
6	0.528404	-1.179084	-3.840342
6	-0.997725	-0.883313	-3.832815
5	2.491369	-1.213596	1.433745
5	1.933716	1.977884	1.483575
5	-1.266313	2.430286	1.521047
5	-0.345831	-2.741961	1.412121
5	-2.706910	-0.501609	1.458949
5	-1.927583	-1.959784	-1.449943
5	1.275590	-2.412577	-1.486252
5	2.714161	0.493795	-1.474720
5	0.347512	2.727852	-1.443504
5	-2.493518	1.228353	-1.438383
5	-0.029135	-0.002963	-2.877702
5	0.031139	-0.045040	2.906449
7	-0.209469	-1.320507	3.768713
7	0.210088	1.271943	-3.788334
6	2.179011	1.812784	3.147642
6	-2.076301	-1.746708	-3.124935
6	-1.080989	2.562499	3.197358

6	1.016053	-2.477011	-3.155574
6	-2.674839	-0.263033	3.146201
6	2.774808	0.261207	-3.160074
6	-0.589435	-2.635207	3.082610
6	0.595773	2.594805	-3.107666
6	2.347498	-1.445800	3.099945
6	-2.439888	1.455002	-3.121630
6	1.258206	-0.643529	3.806320
6	-1.313997	-0.152227	3.844324
5	1.098848	0.891182	3.935879
5	-0.593862	1.212284	3.963350
5	2.070599	-2.779026	2.387332
6	4.075034	-1.217020	1.160396
7	3.448210	-0.506490	2.415191
7	0.602317	-3.392252	2.435212
6	0.098818	-4.246102	1.141077
5	-1.977746	-2.777784	2.417325
5	-3.239777	1.025652	2.461880
6	-3.997366	-1.411397	1.191440
7	-3.043713	-1.619019	2.466223
7	-2.487592	2.436921	2.465818
7	1.577424	3.117123	2.448012
5	-0.030409	3.440290	2.455272
6	-2.576898	3.345657	1.204162
6	2.410259	3.491691	1.165590
5	3.327172	1.117064	2.395008
7	-1.554351	-3.069604	-2.453774
5	-3.279104	-1.067195	-2.407600
6	-2.418833	-3.465976	-1.181614
7	2.455050	-2.385438	-2.482172
5	0.009746	-3.410929	-2.446171
6	2.559539	-3.344146	-1.225968
7	3.089866	1.619989	-2.455212
5	3.287779	-1.008509	-2.440694
6	4.002476	1.429091	-1.189700
6	-0.110266	4.234228	-1.187045
5	1.986574	2.769974	-2.439246
7	-0.613160	3.370180	-2.458422
7	-3.478056	0.523055	-2.395293
5	-2.102602	2.770544	-2.397750
6	-4.084326	1.214236	-1.128035
13	-4.521462	0.447682	0.785109
13	-0.981161	4.431428	0.754442
13	3.937904	2.320514	0.712062
13	3.408853	-3.020145	0.692838
13	-1.827659	-4.155971	0.728863
13	0.973607	-4.440802	-0.796327
13	4.526879	-0.427474	-0.745472
13	1.816247	4.154474	-0.756878
13	-3.418122	3.025652	-0.688815
13	-3.943733	-2.291906	-0.741000

S.7: Optimized structure and energy of CBN cluster with some carbons replaced by Si atoms done at B3LYP/6-31G\* level.

E=

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.862457	1.319500	-0.027624
5	-0.761640	0.393819	1.321556
5	0.862325	-1.319537	0.027622
5	0.761504	-0.393747	-1.321512
5	-0.611711	-1.176345	0.858412
5	0.611705	1.176431	-0.858305
5	-0.612554	-1.213536	-0.781798
5	0.764771	-0.326431	1.322636
5	-0.764840	0.326397	-1.322518
5	0.612432	1.213527	0.781869
5	0.837899	-1.982253	3.556013
5	-0.988576	3.953700	0.850600
5	0.247862	3.827859	-1.686397
5	-0.837801	1.982170	-3.555942
5	-0.363984	-2.818237	-3.058792
5	0.988752	-3.953596	-0.850548
5	0.641951	-0.373740	-4.104141
5	-0.641882	0.373613	4.104162
5	0.364082	2.818276	3.058886
6	1.554349	0.146881	-0.008269
6	-1.554475	-0.146821	0.008463
5	-1.214760	-2.409863	-1.541667
5	-1.224410	-2.338823	1.665495
5	-1.526260	0.747764	2.611366
5	-1.517411	0.618526	-2.639686
5	-1.723971	2.606640	-0.047280
5	1.224305	2.338886	-1.665409
5	1.526145	-0.747790	-2.611283
5	1.723953	-2.606599	0.047318
5	1.517545	-0.618563	2.639712
5	1.214626	2.409797	1.541842
5	3.103514	0.320748	-0.018642
5	-3.103666	-0.320754	0.018423
7	-4.026801	-0.225966	-1.274899
7	4.026864	0.225602	1.274661
5	-0.247720	-3.827699	1.686400
6	-3.951880	-1.609672	-0.685508
5	-4.109527	-1.591779	0.848532
5	-4.278492	-0.035710	1.423447
5	-1.834375	-1.926908	-3.132174
6	-0.342650	-3.797045	-1.770440
7	-1.684192	-3.705051	-0.918655
7	-2.031907	-0.425690	-3.581017



6	-0.759985	0.471397	-4.104865
5	-2.218276	2.237106	-2.497697
5	-2.302080	3.012817	1.583978
6	-1.066227	3.989089	-0.751095
7	-2.344518	3.230741	-1.282952
7	-2.246247	2.070045	2.865319
7	-1.813833	-2.220672	3.068438
5	-1.948246	-0.683500	3.613631
6	-0.868619	1.898228	3.628238
6	-0.398363	-2.897916	3.001284
5	-1.651441	-3.791663	0.705670
7	1.813775	2.220681	-3.068422
5	1.651575	3.791778	-0.705728
6	0.398496	2.897898	-3.001282
7	2.246199	-2.070017	-2.865296
5	1.948342	0.683415	-3.613654
6	0.868745	-1.898301	-3.628116
7	2.344538	-3.230517	1.282993
5	2.302572	-3.012655	-1.583887
6	1.066345	-3.989112	0.751098
6	0.760010	-0.471506	4.104937
5	2.218349	-2.237231	2.497920
7	2.031970	0.425681	3.581022
7	1.684358	3.704893	0.918690
5	1.834423	1.926919	3.132263
6	0.342885	3.797108	1.770427
14	-3.588130	0.606841	-2.983182
14	-3.731683	3.205434	0.090762
14	-3.512136	0.498938	3.206368
14	-3.135833	-3.101273	1.835822
14	-3.181969	-2.907752	-1.929762
14	3.588329	-0.606835	2.983312
14	3.731931	-3.204780	-0.090630
14	3.511916	-0.498303	-3.206460
14	3.135838	3.101075	-1.835768
14	3.181953	2.907454	1.929724
6	3.952034	1.609307	0.685485
5	4.278388	0.035733	-1.423623
5	4.109464	1.591685	-0.848562
14	4.764262	-1.035187	0.083287
14	-4.765009	1.034668	-0.083883

**S.8:** Optimized structure and energy of CBN cluster with some nitrogens replaced by P atoms done at B3LYP/6-31G\* level.

E=

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.127417	1.395394	0.838020

5	1.373699	0.845754	0.213246
5	0.127417	-1.395394	-0.838020
5	-1.373699	-0.845754	-0.213246
5	1.348415	-0.871362	0.212251
5	-1.348415	0.871362	-0.212251
5	-0.160814	-1.392914	0.847922
5	1.081747	-0.012788	-1.226699
5	-1.081747	0.012788	1.226699
5	0.160814	1.392914	-0.847922
5	3.429689	-1.172228	-2.355316
5	-3.197934	1.799214	-2.111523
5	0.233457	4.227013	0.902288
5	-2.373340	3.182994	-1.507356
5	-2.730428	3.345505	0.088829
5	0.224729	-2.786086	3.360112
5	-2.138979	1.580922	3.286131
5	2.373340	-3.182994	1.507356
5	3.197934	-1.799214	2.111523
5	0.465576	2.852363	3.270328
5	-1.327148	-3.547060	-1.927232
5	2.730428	-3.345505	-0.088829
5	-3.429689	1.172228	2.355316
5	-0.224729	2.786086	-3.360112
5	-1.538190	0.115745	4.058009
5	-3.551702	-1.651918	-1.944142
5	-1.860442	-3.508732	1.750199
5	-4.131483	-0.599114	-0.760734
5	-0.233457	-4.227013	-0.902288
5	-4.025581	-1.415242	0.661669
5	1.476764	2.575586	-3.045433
5	4.025581	1.415242	-0.661669
5	-0.465576	-2.852363	-3.270328
5	4.131483	0.599114	0.760734
5	3.551702	1.651918	1.944142
5	1.538190	-0.115745	-4.058009
5	1.073724	-1.395814	3.975989
5	2.138979	-1.580922	-3.286131
5	0.170503	0.012244	4.338690
5	0.996212	1.386148	4.014947
5	-1.476764	-2.575586	3.045433
5	-1.073724	1.395814	-3.975989
5	1.327148	3.547060	1.927232
5	1.860442	3.508732	-1.750199
5	-0.996212	-1.386148	-4.014947
5	-0.170503	-0.012244	-4.338690
6	-0.611274	-0.005603	-1.471258
6	0.611274	0.005603	1.471258
6	-1.137756	0.020572	-2.882270
6	0.143839	-2.675577	-1.636455
6	-2.686269	-1.544099	-0.467654
6	-2.542729	1.729049	-0.514372
6	0.351865	2.624028	-1.709780

6	2.047032	-0.099528	-2.385941
6	-0.143839	2.675577	1.636455
6	-2.047032	0.099528	2.385941
6	-0.351865	-2.624028	1.709780
6	2.542729	-1.729049	0.514372
6	2.686269	1.544099	0.467654
6	1.137756	-0.020572	2.882270
6	-2.397247	0.978807	-3.263120
6	-3.920110	1.026047	-0.952493
6	-0.904088	3.489020	-2.160528
6	2.171704	1.127221	-3.403055
6	1.057757	-2.778067	-2.936679
6	-2.743902	-2.856166	-1.389889
6	0.904088	-3.489020	2.160528
6	3.920110	-1.026047	0.952493
6	2.743902	2.856166	1.389889
6	-1.057757	2.778067	2.936679
6	-2.171704	-1.127221	3.403055
6	2.397247	-0.978807	3.263120
15	-2.781926	-0.831073	-3.541733
15	2.781926	0.831073	3.541733
15	-3.287849	-3.178567	0.407794
15	-4.049067	2.052688	0.654416
15	0.344791	4.482391	-1.073156
15	3.835888	0.708879	-2.503327
15	1.562911	-4.026522	-1.565563
15	4.049067	-2.052688	-0.654416
15	-0.344791	-4.482391	1.073156
15	-3.835888	-0.708879	2.503327
15	-1.562911	4.026522	1.565563
15	3.287849	3.178567	-0.407794

**S.9:** Optimized structures of B84 based stuffed CBN clusters formed from each of the eight pentagonal pyramid isomers calculated at B3LYP/6-31G\* level.

CBN clusters from pentagonal pyramid isomer I

1a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.250955	1.268262	1.123855
5	1.192144	0.928412	0.211674
5	0.250955	-1.268262	-1.123855
5	-1.192144	-0.928412	-0.211674
5	1.483129	-0.739553	0.037216
5	-1.483129	0.739553	-0.037216
5	0.131599	-1.517667	0.746964

5	1.031177	0.323660	-1.360263
5	-1.031177	-0.323660	1.360263
5	-0.131599	1.517667	-0.746964
5	-3.161806	1.840133	-1.968916
5	-2.589853	3.355677	-1.456296
5	0.092370	-2.714606	3.210371
5	-2.585178	1.625980	2.843873
5	2.589853	-3.355677	1.456296
5	3.161806	-1.840133	1.968916
5	1.007800	2.667457	3.149641
5	-1.065094	-3.563510	-1.728940
5	-0.092370	2.714606	-3.210371
5	-1.027881	0.312004	4.421323
5	-3.467173	-1.442257	-1.975770
5	-4.335913	-0.551872	-0.808536
5	1.547843	2.404938	-2.674815
5	-1.007800	-2.667457	-3.149641
5	4.335913	0.551872	0.808536
5	3.467173	1.442257	1.975770
5	1.027881	-0.312004	-4.421323
5	1.132558	-1.364377	3.860785
5	2.585178	-1.625980	-2.843873
5	0.564988	0.054871	4.625724
5	1.562873	1.303715	4.012735
5	-1.547843	-2.404938	2.674815
5	-1.132558	1.364377	-3.860785
5	1.065094	3.563510	1.728940
5	-1.562873	-1.303715	-4.012735
5	-0.564988	-0.054871	-4.625724
6	-0.632748	0.101687	-1.415403
6	0.632748	-0.101687	1.415403
6	2.513201	-0.947545	3.132371
6	2.646066	0.573709	3.118616
6	-2.646066	-0.573709	-3.118616
6	-2.513201	0.947545	-3.132371
6	-2.977251	-2.689914	0.293012
6	2.977251	2.689914	-0.293012
6	-3.580009	1.959743	0.450710
6	3.580009	-1.959743	-0.450710
6	-0.602696	-3.573146	0.693616
6	0.602696	3.573146	-0.693616
6	1.550379	-3.601812	-0.943996
6	-1.550379	3.601812	0.943996
6	-3.307914	-0.327005	1.659938
6	3.307914	0.327005	-1.659938
7	2.082662	-0.474739	-3.650281
7	0.066528	-2.287718	-2.209032
7	-2.460919	-1.500445	-0.508554
7	-2.734149	1.222024	-0.540578
7	-0.324381	2.770672	-1.497296
7	-0.066528	2.287718	2.209032
7	2.460919	1.500445	0.508554

7	2.734149	-1.222024	0.540578
7	0.324381	-2.770672	1.497296
7	-2.082662	0.474739	3.650281
7	1.254647	-0.102574	2.685478
7	-1.254647	0.102574	-2.685478
6	-3.665980	-1.264841	0.490368
5	-2.740841	-2.859844	-1.337215
5	1.509447	-2.791566	-2.232702
5	2.217845	0.829102	-2.665949
5	-1.295016	3.530237	-2.412088
5	-4.265078	1.177859	-0.809560
6	-2.659322	3.278003	0.135977
6	1.857077	3.121533	-1.227878
6	3.448450	-1.109236	-1.706933
6	-0.021915	-3.899196	-0.585785
6	0.021915	3.899196	0.585785
5	-1.509447	2.791566	2.232702
5	2.740841	2.859844	1.337215
6	3.665980	1.264841	-0.490368
6	2.659322	-3.278003	-0.135977
5	4.265078	-1.177859	0.809560
5	1.295016	-3.530237	2.412088
6	-1.857077	-3.121533	1.227878
6	-3.448450	1.109236	1.706933
5	-2.217845	-0.829102	2.665949

1b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.100365	1.392735	0.810863
5	1.361629	0.816548	0.170268
5	0.100365	-1.392735	-0.810863
5	-1.361629	-0.816548	-0.170268
5	1.318886	-0.876309	0.185144
5	-1.318886	0.876309	-0.185144
5	-0.166878	-1.371696	0.833096
5	1.052945	-0.034830	-1.219509
5	-1.052945	0.034830	1.219509
5	0.166878	1.371696	-0.833096
5	3.529751	-1.111745	-2.224604
5	0.085653	4.256178	0.786789
5	-2.323885	3.148532	-1.410812
5	-2.742028	3.288551	0.259221
5	-2.179057	1.552156	3.206967
5	2.323885	-3.148532	1.410812
5	-1.248107	-3.543909	-1.833647
5	2.742028	-3.288551	-0.259221
5	-3.529751	1.111745	2.224604
5	-1.869730	-3.542349	1.549261

5	-4.051097	-0.594796	-0.709316
5	-0.085653	-4.256178	-0.786789
5	-3.962746	-1.501170	0.747742
5	1.491507	2.567697	-2.927802
5	3.962746	1.501170	-0.747742
5	4.051097	0.594796	0.709316
5	0.967287	-1.351993	3.721270
5	2.179057	-1.552156	-3.206967
5	0.092827	0.055201	4.135340
5	1.067588	1.379197	3.676467
5	-1.491507	-2.567697	2.927802
5	-0.967287	1.351993	-3.721270
5	1.248107	3.543909	1.833647
5	1.869730	3.542349	-1.549261
5	-1.067588	-1.379197	-3.676467
5	-0.092827	-0.055201	-4.135340
6	-0.571085	0.001247	-1.334745
6	0.571085	-0.001247	1.334745
6	2.354192	-0.833496	2.995514
6	2.415046	0.735071	2.968194
6	-2.415046	-0.735071	-2.968194
6	-2.354192	0.833496	-2.995514
6	-2.680751	-2.823982	-1.276638
6	2.680751	2.823982	1.276638
6	-3.882741	1.062772	-0.768173
6	3.882741	-1.062772	0.768173
6	0.795667	-3.534258	1.993848
6	-0.795667	3.534258	-1.993848
6	1.112472	-2.829690	-2.781064
6	-1.112472	2.829690	2.781064
6	-2.298150	-1.091759	3.245759
6	2.298150	1.091759	-3.245759
7	1.923121	-0.115727	-2.293514
7	0.117875	-2.571459	-1.541919
7	-2.581948	-1.431551	-0.405576
7	-2.442601	1.639816	-0.460580
7	0.324872	2.498823	-1.626892
7	-0.117875	2.571459	1.541919
7	2.581948	1.431551	0.405576
7	2.442601	-1.639816	0.460580
7	-0.324872	-2.498823	1.626892
7	-1.923121	0.115727	2.293514
7	1.060389	-0.001716	2.592855
7	-1.060389	0.001716	-2.592855
5	3.562254	0.616445	-2.290563
6	1.534971	-0.159224	-3.800663
6	-0.147846	2.651607	-3.104808
6	-3.034924	1.734496	-1.894818
6	-3.210740	-1.464126	-1.826789
6	-0.434330	-2.738885	-2.993793
5	0.358164	4.169858	-0.999195
5	-3.773644	1.953839	0.624412

5	-3.078888	-2.928009	0.324095
5	1.431602	-3.753207	-1.445222
5	-3.562254	-0.616445	2.290563
6	-1.534971	0.159224	3.800663
5	-1.431602	3.753207	1.445222
6	0.434330	2.738885	2.993793
6	3.210740	1.464126	1.826789
5	3.078888	2.928009	-0.324095
5	3.773644	-1.953839	-0.624412
6	3.034924	-1.734496	1.894818
6	0.147846	-2.651607	3.104808
5	-0.358164	-4.169858	0.999195

1c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-1.071475	0.824072	0.833020
5	-0.514124	-0.647214	1.356101
5	1.071475	-0.824072	-0.833020
5	0.514124	0.647214	-1.356101
6	-0.164685	-1.495948	0.000000
5	-1.494723	-0.555063	0.000000
6	0.164685	1.495948	0.000000
5	1.494723	0.555063	0.000000
5	-0.514124	-0.647214	-1.356101
5	1.071475	-0.824072	0.833020
5	-1.071475	0.824072	-0.833020
5	0.514124	0.647214	1.356101
5	2.004908	3.848700	0.000000
6	-2.566132	1.058048	-2.947079
6	-0.623519	3.868596	0.785615
6	-0.623519	3.868596	-0.785615
5	-2.004908	-3.848700	0.000000
6	2.566132	-1.058048	-2.947079
6	0.623519	-3.868596	0.785615
6	0.623519	-3.868596	-0.785615
6	2.469193	1.801269	2.675239
6	2.469193	1.801269	-2.675239
6	1.235692	2.771503	-2.668704
5	0.004898	2.128873	-3.560891
5	-0.004898	-2.128873	3.560891
6	1.235692	2.771503	2.668704
6	-1.235692	-2.771503	2.668704
6	-2.469193	-1.801269	2.675239
5	-0.004898	-2.128873	-3.560891
5	-3.381552	-2.772526	0.000000
5	0.004898	2.128873	3.560891
6	-3.956793	-0.234197	-0.781930
6	-3.956793	-0.234197	0.781930
5	3.381552	2.772526	0.000000

6	-2.566132	1.058048	2.947079
6	3.956793	0.234197	-0.781930
6	2.566132	-1.058048	2.947079
6	3.956793	0.234197	0.781930
5	-0.923890	-3.753330	1.317970
5	-0.923890	-3.753330	-1.317970
5	-3.529986	-1.716973	1.332062
5	-3.529986	-1.716973	-1.332062
5	-0.548688	-0.687010	4.281142
5	-2.075054	-0.472697	3.545299
6	1.590463	-2.278739	2.953469
5	0.923890	3.753330	1.317970
5	0.923890	3.753330	-1.317970
5	3.529986	1.716973	-1.332062
5	3.529986	1.716973	1.332062
5	0.548688	0.687010	-4.281142
5	2.075054	0.472697	-3.545299
5	0.548688	0.687010	4.281142
5	1.937299	-3.241033	1.666859
5	3.341590	-2.678292	0.879556
5	3.589870	-1.186004	1.665480
5	3.341590	-2.678292	-0.879556
5	1.937299	-3.241033	-1.666859
5	3.589870	-1.186004	-1.665480
6	1.590463	-2.278739	-2.953469
5	-0.548688	-0.687010	-4.281142
5	-2.075054	-0.472697	-3.545299
6	-2.469193	-1.801269	-2.675239
6	-1.235692	-2.771503	-2.668704
5	2.075054	0.472697	3.545299
5	-3.589870	1.186004	1.665480
5	-1.937299	3.241033	1.666859
5	-3.341590	2.678292	0.879556
6	-1.590463	2.278739	2.953469
6	-1.590463	2.278739	-2.953469
5	-1.937299	3.241033	-1.666859
5	-3.341590	2.678292	-0.879556
5	-3.589870	1.186004	-1.665480
7	-0.377448	-2.837338	0.000000
7	0.377448	2.837338	0.000000
7	-2.001082	1.611532	-1.493833
7	-2.001082	1.611532	1.493833
7	0.929274	1.197665	2.557772
7	2.760733	1.128543	0.000000
7	0.929274	1.197665	-2.557772
7	2.001082	-1.611532	-1.493833
7	-0.929274	-1.197665	-2.557772
7	-2.760733	-1.128543	0.000000
7	-0.929274	-1.197665	2.557772
7	2.001082	-1.611532	1.493833



Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	1.556062	0.339746	-0.085450
5	0.983229	-0.938543	0.834545
5	-1.549759	-0.339769	0.107631
5	-0.974212	0.923881	-0.807632
5	-0.528433	-0.525053	1.412532
5	0.672950	0.643633	1.296936
5	0.528457	0.514362	-1.382070
5	-0.661705	-0.628327	-1.270390
5	-0.892384	1.011830	0.848056
5	0.893767	-0.993976	-0.822663
5	-1.360196	-3.763066	1.624557
5	-0.113038	2.015456	-3.648374
5	3.942414	-0.402150	-1.167337
5	-3.600821	-1.194130	1.783814
5	1.322157	2.586971	-2.916086
5	2.379836	3.498675	-0.326677
5	0.096440	-2.028507	3.668732
5	-1.382515	-2.673945	3.044951
5	-2.192771	1.451846	3.170446
5	-3.549743	1.560547	-1.402712
5	1.533467	3.876320	1.119656
5	-1.609693	3.425633	-1.628754
5	1.285846	-3.530084	-1.680874
5	2.940329	-2.912445	0.663645
5	1.713139	-3.525611	1.685693
5	-2.386001	-3.514141	0.269267
5	-1.386480	3.646055	1.738091
5	2.428756	0.273594	3.314769
5	-3.075874	-1.559507	-2.359407
7	-1.309096	-1.161000	-2.369972
7	1.598957	-1.870420	-1.627798
7	-0.722726	-2.820494	0.165620
7	-2.896493	-0.640213	0.242852
7	-1.850774	1.762045	-1.472511
7	0.731436	2.821767	-0.154880
7	-1.608713	1.913502	1.619267
7	1.338033	1.211345	2.369857
7	1.865886	-1.801895	1.466406
7	2.896523	0.643672	-0.271055
7	0.893649	0.977595	-2.633831
7	-0.920687	-1.033961	2.638840
6	-3.185077	1.697404	1.896294
6	2.422471	1.373038	-2.989241
6	3.171531	-1.738969	-1.874711
6	-1.420204	-3.631240	-1.047921
6	-2.679922	1.315035	-2.770812
6	1.251644	3.518727	-1.521055
6	0.380419	1.497963	-0.090260

6	-0.378328	-1.497358	0.078412
5	-2.911371	2.942726	-0.608620
6	-1.581620	2.395731	-2.902962
6	-2.700906	2.918710	1.076316
5	-0.969022	2.652925	3.097121
5	-0.085177	4.206332	0.650437
6	-0.144081	3.919413	-0.963854
6	2.673888	-1.310980	2.771836
5	0.954634	-2.626154	-3.096739
6	0.044058	-3.979741	-0.646117
5	0.191197	-4.129356	0.985435
5	-2.439162	-0.281133	-3.311626
5	-1.846097	-2.767515	-2.430118
6	-0.652461	-2.189304	-3.386493
6	-0.977453	-0.761306	-3.883673
6	-3.833504	-1.217465	-0.881207
5	-3.937080	0.372154	1.178372
5	0.234885	0.407729	-4.102477
6	1.789370	0.122409	-3.650642
6	-1.777867	-0.112884	3.652315
6	2.662924	-2.932371	-1.026835
5	2.198441	-1.460735	-3.168891
5	3.566223	-1.523923	1.419311
6	1.598603	-2.428059	2.913340
6	-2.420772	-1.383568	3.026940
5	-0.231518	-0.406125	4.091926
5	-3.621459	-2.230940	0.398158
6	-4.043320	0.257281	-0.447600
6	0.972605	0.760919	3.875368
6	0.667990	2.210912	3.407324
5	3.064669	1.570056	2.398695
5	1.921828	2.859898	2.540780
5	3.611086	1.147613	-1.779946
5	3.611964	2.221214	-0.444124
6	4.042816	-0.224942	0.454782
6	3.825816	1.256662	0.876705

CBN clusters from pentagonal pyramid isomer II

2a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.086238	1.330947	0.830659
5	1.382998	0.646771	0.469210
5	0.086238	-1.330947	-0.830659
5	-1.382998	-0.646771	-0.469210
5	1.145348	-0.994895	0.412840
5	-1.145348	0.994895	-0.412840
5	-0.458629	-1.329648	0.751421

5	1.225006	-0.119920	-1.011991
5	-1.225006	0.119920	1.011991
5	0.458629	1.329648	-0.751421
5	3.646280	-1.300658	-1.663960
5	0.314263	4.063028	1.022707
5	-2.420894	3.420152	-0.072552
5	2.420894	-3.420152	0.072552
5	-3.646280	1.300658	1.663960
5	-2.318505	-3.341425	1.102015
5	-0.314263	-4.063028	-1.022707
5	-4.057812	-1.157757	0.022439
5	4.057812	1.157757	-0.022439
5	0.270375	-1.538663	3.958828
5	-0.512393	-0.056676	4.225027
5	-0.270375	1.538663	-3.958828
5	2.318505	3.341425	-1.102015
5	0.512393	0.056676	-4.225027
6	-0.330074	0.097474	-1.509667
6	0.330074	-0.097474	1.509667
6	1.766955	-1.142588	3.503503
6	-1.766955	1.142588	-3.503503
7	2.281783	-0.240784	-1.893449
7	0.171943	-2.502942	-1.553889
7	-2.576381	-1.202019	-0.896080
7	-2.144865	1.876890	-0.768311
7	0.844281	2.486659	-1.400904
7	-0.171943	2.502942	1.553889
7	2.576381	1.202019	0.896080
7	2.144865	-1.876890	0.768311
7	-0.844281	-2.486659	1.400904
7	-2.281783	0.240784	1.893449
7	0.601005	-0.195902	2.858026
7	-0.601005	0.195902	-2.858026
5	2.050126	0.433082	3.618264
6	0.601706	1.064167	3.898594
6	-0.601706	-1.064167	-3.898594
5	-2.050126	-0.433082	-3.618264
6	1.801378	-3.257090	1.586969
6	3.594885	-1.338166	1.325735
5	2.563865	-2.039305	2.384660
5	3.601060	-2.162262	-0.092653
5	-0.564319	-2.777114	3.078497
5	-0.807980	-4.076457	0.699728
6	0.210920	-3.592908	1.886757
6	-2.063595	-2.493222	2.480842
6	-2.835363	-1.032250	2.743717
6	-2.500086	1.541174	2.806772
5	-2.116493	0.163040	3.605878
5	-3.863430	-0.412943	1.627223
5	0.175793	2.483780	3.195619
5	-1.353191	3.727969	1.353763
6	1.178078	3.236013	2.145085

6	-1.358555	2.729607	2.661260
6	3.834257	0.296686	1.350995
6	2.637036	2.563807	1.757903
5	3.120633	1.197548	2.507111
5	3.261511	2.666046	0.248532
5	-3.261511	-2.666046	-0.248532
5	-3.120633	-1.197548	-2.507111
6	-2.637036	-2.563807	-1.757903
6	-3.834257	-0.296686	-1.350995
6	-1.178078	-3.236013	-2.145085
6	1.358555	-2.729607	-2.661260
5	1.353191	-3.727969	-1.353763
5	-0.175793	-2.483780	-3.195619
5	3.863430	0.412943	-1.627223
5	2.116493	-0.163040	-3.605878
6	2.835363	1.032250	-2.743717
6	2.500086	-1.541174	-2.806772
6	-0.210920	3.592908	-1.886757
6	2.063595	2.493222	-2.480842
5	0.807980	4.076457	-0.699728
5	0.564319	2.777114	-3.078497
5	-3.601060	2.162262	0.092653
5	-2.563865	2.039305	-2.384660
6	-3.594885	1.338166	-1.325735
6	-1.801378	3.257090	-1.586969

2b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.088202	1.329842	0.827004
5	1.380621	0.651413	0.465207
5	0.088202	-1.329842	-0.827004
5	-1.380621	-0.651413	-0.465207
5	1.145506	-0.990511	0.408316
5	-1.145506	0.990511	-0.408316
5	-0.454985	-1.330900	0.751379
5	1.225274	-0.115504	-1.011898
5	-1.225274	0.115504	1.011898
5	0.454985	1.330900	-0.751379
5	-2.586933	1.611778	2.814019
5	1.827235	-3.367369	1.554636
5	-1.212592	-3.346086	-2.126264
5	-3.934283	-0.295082	-1.314800
5	2.156726	2.555148	-2.483889
5	3.934283	0.295082	1.314800
5	0.300199	-1.570653	3.923158
5	2.586933	-1.611778	-2.814019
5	-0.542066	-0.095007	4.196061
5	-2.156726	-2.555148	2.483889

5	-0.300199	1.570653	-3.923158
5	1.212592	3.346086	2.126264
5	0.542066	0.095007	-4.196061
6	-0.331110	0.096263	-1.509714
6	0.331110	-0.096263	1.509714
6	1.803920	-1.122378	3.481755
6	-1.803920	1.122378	-3.481755
7	2.272922	-0.253649	-1.909632
7	0.152581	-2.496497	-1.565434
7	-2.578991	-1.191410	-0.913159
7	-2.131894	1.881189	-0.785177
7	0.840681	2.481024	-1.423510
7	-0.152581	2.496497	1.565434
7	2.578991	1.191410	0.913159
7	2.131894	-1.881189	0.785177
7	-0.840681	-2.481024	1.423510
7	-2.272922	0.253649	1.909632
7	0.603237	-0.193031	2.846406
7	-0.603237	0.193031	-2.846406
5	2.038917	0.484330	3.601110
6	0.555808	1.076292	3.892936
6	-0.555808	-1.076292	-3.892936
5	-2.038917	-0.484330	-3.601110
6	-2.244552	-3.265868	1.024268
6	0.179650	-3.680091	1.861231
5	-0.825222	-3.951659	0.627953
5	-0.558293	-2.882478	3.083010
5	-3.769123	-0.367379	1.520726
5	-2.207396	0.129760	3.629392
6	-3.566894	1.248803	1.579022
6	-2.927494	-1.032355	2.734723
6	-1.383859	2.813094	2.645750
6	0.272970	3.965291	0.958936
5	0.125102	2.559917	3.223773
5	-1.301777	3.643760	1.253004
5	3.171961	2.570190	0.175938
5	3.178590	1.281463	2.515328
6	2.702101	2.618349	1.721014
6	3.932201	1.152966	-0.056641
6	3.649970	-1.389204	1.282998
6	2.370453	-3.320568	0.022946
5	2.653940	-2.069362	2.375723
5	3.472911	-2.125024	-0.151303
5	0.825222	3.951659	-0.627953
6	2.244552	3.265868	-1.024268
6	-0.179650	3.680091	-1.861231
5	0.558293	2.882478	-3.083010
5	-3.472911	2.125024	0.151303
6	-2.370453	3.320568	-0.022946
6	-3.649970	1.389204	-1.282998
5	-2.653940	2.069362	-2.375723
5	-1.827235	3.367369	-1.554636

5	-3.171961	-2.570190	-0.175938
5	-3.178590	-1.281463	-2.515328
6	-3.932201	-1.152966	0.056641
6	-2.702101	-2.618349	-1.721014
6	-0.272970	-3.965291	-0.958936
6	1.383859	-2.813094	-2.645750
5	1.301777	-3.643760	-1.253004
5	-0.125102	-2.559917	-3.223773
5	3.769123	0.367379	-1.520726
6	3.566894	-1.248803	-1.579022
6	2.927494	1.032355	-2.734723
5	2.207396	-0.129760	-3.629392

2d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.090661	1.357934	0.816080
5	1.403487	0.657619	0.446872
5	0.090661	-1.357934	-0.816080
5	-1.403487	-0.657619	-0.446872
5	1.158965	-1.012795	0.391893
5	-1.158965	1.012795	-0.391893
5	-0.475286	-1.351120	0.740082
5	1.254961	-0.127441	-1.004866
5	-1.254961	0.127441	1.004866
5	0.475286	1.351120	-0.740082
5	3.656253	-1.238334	-1.567410
5	0.228313	4.044040	0.932046
5	-1.890534	3.423192	-1.607278
5	-2.437344	3.354355	0.030214
5	-2.643385	1.630119	2.902909
5	1.890534	-3.423192	1.607278
5	-1.219129	-3.413143	-2.196239
5	2.437344	-3.354355	-0.030214
5	-3.656253	1.238334	1.567410
5	-2.268875	-3.344272	0.984713
5	-4.018222	-0.314576	-1.370207
5	-0.228313	-4.044040	-0.932046
5	-3.985814	-1.210272	0.100754
5	2.179803	2.618321	-2.550686
5	3.985814	1.210272	-0.100754
5	4.018222	0.314576	1.370207
5	0.212377	-1.558056	3.746885
5	2.643385	-1.630119	-2.902909
5	-0.592470	-0.037749	4.018628
5	-2.179803	-2.618321	2.550686
5	-0.212377	1.558056	-3.746885
5	1.219129	3.413143	2.196239
5	2.268875	3.344272	-0.984713

5	0.592470	0.037749	-4.018628
6	-0.312924	0.091482	-1.426726
6	0.312924	-0.091482	1.426726
6	1.765990	-1.168078	3.339093
6	-1.765990	1.168078	-3.339093
6	-3.209982	-2.596476	-0.214781
6	3.209982	2.596476	0.214781
6	-3.520099	2.147420	0.127277
6	3.520099	-2.147420	-0.127277
6	-0.821780	-3.999270	0.664334
6	0.821780	3.999270	-0.664334
6	1.313747	-3.679583	-1.293503
6	-1.313747	3.679583	1.293503
6	-3.803806	-0.374404	1.567236
6	3.803806	0.374404	-1.567236
7	2.295214	-0.273619	-1.915887
7	0.147551	-2.520797	-1.568044
7	-2.604692	-1.192664	-0.902246
7	-2.146123	1.900946	-0.787170
7	0.853136	2.502711	-1.421109
7	-0.147551	2.520797	1.568044
7	2.604692	1.192664	0.902246
7	2.146123	-1.900946	0.787170
7	-0.853136	-2.502711	1.421109
7	-2.295214	0.273619	1.915887
7	0.582801	-0.184692	2.743060
7	-0.582801	0.184692	-2.743060
5	2.033250	0.462564	3.408977
6	0.554396	1.121532	3.748651
6	-0.554396	-1.121532	-3.748651
5	-2.033250	-0.462564	-3.408977
5	3.719039	-1.411017	1.307019
6	2.588713	-2.100337	2.275589
6	-2.588713	2.100337	-2.275589
5	-3.719039	1.411017	-1.307019
5	2.742927	2.658984	1.769118
6	3.131369	1.207901	2.395212
6	-3.131369	-1.207901	-2.395212
5	-2.742927	-2.658984	-1.769118
5	-1.412682	2.861326	2.695878
6	0.157873	2.571976	3.103404
6	-0.157873	-2.571976	-3.103404
5	1.412682	-2.861326	-2.695878
5	-2.967406	-1.050056	2.795050
6	-2.183254	0.193050	3.501539
6	2.183254	-0.193050	-3.501539
5	2.967406	1.050056	-2.795050
5	0.192186	-3.740199	1.908738
6	-0.619819	-2.807093	2.967530
6	0.619819	2.807093	-2.967530
5	-0.192186	3.740199	-1.908738

2e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	1.462364	0.157021	-0.616620
5	1.143507	0.418790	0.998146
5	-1.461606	-0.141670	0.620867
5	-1.153892	-0.425123	-1.002752
5	-0.400703	1.032832	1.146947
5	0.559311	1.482564	-0.147572
5	0.400418	-1.013771	-1.132149
5	-0.554911	-1.458285	0.156096
5	-1.046434	1.112859	-0.390333
5	1.060726	-1.121168	0.386816
5	-0.567621	-0.139065	4.196930
5	4.013369	-0.772587	-0.822912
5	-3.289432	0.852981	2.374850
5	0.913213	-1.446712	-3.747692
5	1.662725	1.317800	-3.671002
5	-1.796699	3.228197	1.908961
5	3.472633	1.855680	-1.310567
5	-0.966552	0.727266	-3.986082
5	0.445990	2.514364	3.263236
5	-4.113654	-0.660820	0.261768
5	-0.874129	1.577461	3.853511
5	-2.548523	3.268645	0.288009
5	-3.775583	-1.066671	-1.422096
5	0.737618	2.682317	-3.191223
5	-3.302062	1.698760	-1.822171
5	-1.866537	-1.978979	-3.124071
5	-2.289408	-0.365679	-3.560558
5	2.065859	-2.945157	2.256881
5	3.391979	-0.385141	2.343149
5	2.218293	0.210457	3.471408
5	2.914524	2.272438	1.893162
5	-1.660597	-1.347531	3.652157
5	1.223275	3.657753	-1.788531
5	-2.017972	2.764181	-2.296903
5	2.239552	3.428003	0.711937
5	-0.789969	-3.996471	-0.807444
5	3.128979	0.925447	-2.740464
5	-2.674334	-3.016634	0.940565
5	0.859650	-2.292068	3.369965
7	-1.067993	-2.732823	0.307176
7	1.947041	-2.126550	0.750030
7	-0.192509	-1.041838	2.719455
7	-2.729623	-0.270852	1.162734
7	-2.127868	-0.819161	-1.911883
7	0.201931	1.076618	-2.704088
7	-1.969521	2.069034	-0.762225
7	1.016321	2.781813	-0.306650



7	2.154292	0.743364	1.881270
7	2.721158	0.334201	-1.169965
7	0.755998	-1.897907	-2.132200
7	-0.708310	1.914214	2.170294
6	-0.178584	3.452823	2.085205
6	-2.144652	2.008757	2.906818
6	-1.626161	3.652182	-0.981679
6	-3.485730	2.009643	-0.228602
6	0.916430	-0.759369	3.904561
6	-0.718704	-2.557374	3.096498
6	-3.351483	0.111853	-2.426254
6	-2.769809	-2.308612	-1.802452
6	0.558975	0.171469	-4.034841
6	-0.819862	2.203905	-3.331479
6	2.493409	3.185746	-0.862823
6	1.987661	1.792558	3.125051
6	3.674237	0.904385	1.376181
6	0.667680	3.898946	0.809877
5	-0.006961	4.091403	-0.661876
6	3.959367	0.743009	-0.201482
6	3.386775	-0.622630	-2.291192
6	-2.259035	-3.271255	-0.623749
6	-3.854699	0.858664	0.837651
6	0.093076	0.565953	-1.439332
6	-0.092998	-0.560175	1.442565
6	-0.252509	-2.490100	-3.266397
6	1.842302	-3.054449	-1.870458
5	2.347170	-1.847279	-2.854137
5	0.289809	-3.535143	-2.162869
5	-3.114550	-0.832059	2.768712
6	-3.543350	-1.629148	1.411296
6	-0.183010	-4.048342	0.685548
5	-1.242214	-3.491517	1.799627
5	1.481590	-3.767222	0.857493
5	3.556633	-2.173049	0.147359
6	2.402667	-3.220640	-0.372697
6	3.234564	-1.954112	1.707137

2f

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	1.006921	-0.000652	1.193901
5	0.891070	-1.300251	0.171877
5	-1.035508	0.011386	-1.195206
5	-0.900255	1.330110	-0.167616
5	-0.706356	-1.383122	-0.329084
5	-0.359870	-0.938160	1.231630
5	0.701763	1.392997	0.350458
5	0.352901	0.927845	-1.191931
5	-1.533331	-0.122431	0.375497

5	1.575854	0.141230	-0.365676
5	0.268019	-2.879086	-3.058007
5	0.555326	4.192730	0.527173
5	3.554383	0.112648	1.923399
5	2.951907	2.936224	0.366173
5	-2.730291	-1.478248	-2.642538
5	0.911285	3.459415	2.058020
5	0.069637	1.519921	3.939015
5	-2.916416	-2.966519	-0.255151
5	1.711008	-0.998821	3.618761
5	-1.855365	2.792976	2.482263
5	-0.459469	-4.099919	-0.417114
5	-3.078261	1.223604	-2.657985
5	-0.940137	-3.635194	-1.998696
5	-3.821411	-1.601029	0.435352
5	-2.830340	2.624418	-1.629285
5	-1.343513	0.553274	3.968246
5	-3.953460	1.124187	0.485269
5	-1.107750	4.114974	-0.114553
5	-2.336140	3.467318	0.900207
5	3.684109	-0.408212	-2.134922
5	3.446088	-2.520600	-0.015252
5	2.270539	-3.319106	-0.996617
5	3.846364	1.658658	-0.425627
5	-1.822557	0.842340	-3.738108
5	1.467047	-3.560564	1.561064
5	-0.138366	-1.401983	-3.827415
5	-1.225579	-1.207845	3.876477
5	-3.532039	0.519673	2.058717
5	0.125166	-3.196212	2.651649
5	2.286029	1.991729	-2.789878
5	1.404299	3.274225	-2.049217
5	4.146860	-1.018665	-0.602346
5	1.666576	0.737448	3.803567
5	-0.328855	1.859075	-3.684775
5	2.463901	-1.272496	-3.071154
7	0.677330	1.731130	-2.261000
7	2.924518	0.209814	-0.738988
7	0.812188	-1.316096	-2.416543
7	-1.919617	0.024372	-2.269566
7	-1.661846	2.483241	-0.319435
7	-0.852029	1.306103	2.467325
7	-2.871766	-0.217720	0.699063
7	-0.695473	-1.731736	2.316853
7	1.686911	-2.429003	0.291615
7	1.859883	-0.005961	2.273945
7	1.278768	2.609799	0.670262
7	-1.262770	-2.616819	-0.645470
6	-1.669946	-3.635643	0.568363
6	-2.371236	-2.874744	-1.774404
6	-3.465311	-1.108238	1.933098
6	-4.007807	-0.224105	-0.441450

6	2.361903	2.696378	1.875040
6	1.762423	3.703153	-0.430409
6	4.107934	0.275020	0.364114
6	3.473708	1.187459	-1.924030
6	1.788467	-2.652718	-2.510333
6	1.200086	-0.463878	-3.752751
6	-3.262641	2.555780	-0.080084
6	-1.408670	3.448498	-1.587319
6	-0.299103	2.774987	2.969915
6	-2.402248	1.346491	2.998051
6	0.238189	-1.923684	3.643168
6	1.157765	-3.951289	0.023662
6	2.756357	-2.561960	1.465697
6	-1.413874	-3.165659	2.076628
5	-2.305734	-2.013289	2.795615
6	2.872455	-1.288311	2.480263
6	2.722138	1.296930	2.669251
6	1.159583	1.154433	-3.649905
6	-0.156205	3.078296	-2.575826
6	-1.665911	-0.778306	-3.652689
6	-3.511336	-0.206995	-1.978299
6	-0.472040	0.717970	1.294584
6	0.453166	-0.693180	-1.263891

CBN clusters from pentagonal pyramid isomer III

3a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.285687	1.294461	0.970732
5	1.305406	0.978346	0.270024
5	0.285687	-1.294461	-0.970732
5	-1.305406	-0.978346	-0.270024
5	1.467127	-0.740987	0.175849
5	-1.467127	0.740987	-0.175849
5	-0.059788	-1.341172	0.820866
5	1.267655	0.129618	-1.254239
5	-1.267655	-0.129618	1.254239
5	0.059788	1.341172	-0.820866
5	2.829244	-1.196828	-2.479674
5	0.434823	4.050378	1.090737
5	-2.586622	3.291694	-0.060189
5	-2.829244	1.196828	2.479674
5	-1.891251	-2.973710	2.060029
5	-0.434823	-4.050378	-1.090737
5	-3.729207	-1.541539	0.200706
5	3.729207	1.541539	-0.200706
5	1.216320	1.238293	4.194943
5	-1.216320	-1.238293	-4.194943

6	-0.709224	-0.015557	-1.502863
6	0.709224	0.015557	1.502863
7	0.255473	0.052831	4.614862
7	-0.255473	-0.052831	-4.614862
5	2.586622	-3.291694	0.060189
6	3.120973	-1.640637	2.348197
6	-3.120973	1.640637	-2.348197
6	3.238606	1.477111	2.400058
6	-3.238606	-1.477111	-2.400058
6	0.629260	2.514943	3.537062
6	-0.629260	-2.514943	-3.537062
6	-1.019132	0.197589	4.225642
6	1.019132	-0.197589	-4.225642
6	0.383157	-2.227151	3.391080
6	-0.383157	2.227151	-3.391080
5	2.724292	0.800409	3.725418
5	2.637878	-0.829713	3.594188
6	1.069744	-1.064844	3.919281
6	-1.069744	1.064844	-3.919281
5	-2.724292	-0.800409	-3.725418
5	-2.637878	0.829713	-3.594188
5	2.307202	-2.814085	1.698335
5	3.202917	-2.195691	-1.095374
7	3.681508	-0.927218	1.289263
7	0.894425	-2.961388	2.341277
5	-1.159974	-2.219759	3.349588
5	-1.298012	-3.470202	0.380270
5	-1.635334	1.562556	3.604491
5	-3.101276	-1.491657	1.677736
7	-1.696358	-0.846391	3.644976
7	-0.678871	2.524855	3.168147
5	-1.192056	3.780423	0.781869
5	1.309451	3.241777	2.354427
5	2.966674	2.924710	-0.819726
5	3.870820	0.580109	1.195166
7	2.526580	2.481125	1.858837
5	-2.307202	2.814085	-1.698335
7	-3.681508	0.927218	-1.289263
5	-3.202917	2.195691	1.095374
7	1.696358	0.846391	-3.644976
5	1.635334	-1.562556	-3.604491
5	3.101276	1.491657	-1.677736
5	1.298012	3.470202	-0.380270
5	1.891251	2.973710	-2.060029
5	1.159974	2.219759	-3.349588
7	-0.894425	2.961388	-2.341277
7	-2.526580	-2.481125	-1.858837
5	-3.870820	-0.580109	-1.195166
5	-2.966674	-2.924710	0.819726
5	-1.309451	-3.241777	-2.354427
5	1.192056	-3.780423	-0.781869
7	0.678871	-2.524855	-3.168147

6	1.420906	0.003725	2.820570
6	-2.500680	-0.348545	2.479681
6	-0.457674	2.652365	1.680757
6	2.293409	2.190588	0.449787
6	2.776209	-1.494474	0.233821
6	-0.312632	-2.696202	1.460388
6	-2.293409	-2.190588	-0.449787
6	0.457674	-2.652365	-1.680757
6	2.500680	0.348545	-2.479681
6	0.312632	2.696202	-1.460388
6	-2.776209	1.494474	-0.233821
6	-1.420906	-0.003725	-2.820570

3b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	1.372702	-0.480470	0.776529
5	-0.161285	-1.165136	1.283885
5	-1.372763	0.480458	-0.776439
5	0.161207	1.165152	-1.283690
5	-1.358816	0.043454	0.901116
5	1.358703	-0.043477	-0.901011
5	-0.633075	1.525221	0.363548
5	-1.103556	-1.177884	-0.239686
5	1.103532	1.177880	0.239776
5	0.633021	-1.525262	-0.363412
5	2.651690	0.141495	3.381614
5	-2.651711	-0.141511	-3.381601
6	-0.182003	-0.503996	-1.494335
6	0.181971	0.503982	1.494413
5	-1.216198	2.997465	0.965508
5	-2.900168	-0.234790	1.501149
5	-0.488225	-3.684830	1.834467
5	2.258151	2.274356	0.667206
5	2.860225	-0.847320	1.353287
5	2.899830	0.234788	-1.501274
5	0.488556	3.684724	-1.834406
5	-2.860249	0.847258	-1.353328
5	-2.258249	-2.274276	-0.667110
5	1.216355	-2.997446	-0.965423
5	-0.457962	-1.211922	-2.938833
5	0.457940	1.211921	2.938856
7	1.934215	1.313184	3.305041
7	-1.934239	-1.313206	-3.305002
5	-0.838592	-1.019344	3.679611
5	-1.492050	0.476197	3.920773
6	-0.854894	1.780845	3.523440
6	0.854769	-1.781121	-3.523421
5	0.838919	1.019001	-3.679528
5	1.491881	-0.476534	-3.920839

5	-3.651530	1.240330	2.037814
5	0.149353	4.072549	1.271572
5	3.888222	1.721123	1.434634
5	3.158506	-2.585342	2.157313
5	-2.142769	-2.856759	2.182823
5	3.651299	-1.240202	-2.037902
5	-3.888234	-1.721142	-1.434684
5	-0.149118	-4.072360	-1.271766
5	2.142963	2.857274	-2.182872
5	-3.158571	2.585290	-2.157363
5	2.597635	2.370063	2.373974
5	-0.571721	-2.213801	2.699034
5	3.560646	-1.071519	2.867598
5	-2.969289	-0.108730	3.201210
5	-1.460757	2.793441	2.614734
5	1.460535	-2.793663	-2.614675
5	-2.597651	-2.370087	-2.373969
5	-3.560688	1.071489	-2.867636
5	0.572020	2.213434	-2.698804
5	2.968950	0.109122	-3.201339
6	2.078603	3.796012	0.157180
7	3.829183	2.192681	0.066717
5	1.807149	3.787528	1.594107
5	4.377385	-0.010410	1.743761
7	3.557924	-2.896990	0.763488
6	4.223213	-0.529593	0.403197
6	0.792809	-4.185413	1.192467
7	-1.846576	-3.830986	1.185263
5	1.882212	-3.617274	1.943541
5	-3.351216	-1.667863	2.524723
7	-4.152252	0.553068	0.904285
6	-3.848840	-1.832339	1.169218
6	-3.367163	3.152142	0.426429
7	-0.762979	4.250008	0.248272
5	-2.990576	2.817572	1.794739
5	2.990478	-2.817446	-1.794747
6	3.367199	-3.152023	-0.426467
7	0.763145	-4.250163	-0.248449
7	-3.828870	-2.192792	-0.066746
6	-2.078491	-3.796091	-0.157051
5	-1.807062	-3.787400	-1.593948
5	-4.377435	0.010325	-1.743838
7	-3.557895	2.897083	-0.763523
6	-4.223397	0.529660	-0.403307
6	-0.792702	4.185155	-1.192667
7	1.846698	3.831253	-1.185165
5	-1.882288	3.617184	-1.943610
5	3.350939	1.668135	-2.524691
6	3.849140	1.832363	-1.169201
7	4.152032	-0.552804	-0.904434

3c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.571110	1.499474	0.484111
5	-1.597109	0.115223	0.434522
5	0.550837	-1.498951	-0.461794
5	1.586102	-0.113312	-0.422814
5	-0.982778	-0.899256	-0.784126
5	0.972461	0.914509	0.794027
5	0.349793	-0.197085	-1.569249
5	-0.641680	-1.252370	0.782955
5	0.631789	1.266754	-0.772746
5	-0.357522	0.203431	1.585641
5	2.665711	1.082486	2.960230
5	1.304911	2.169995	3.165240
5	1.507158	3.382762	1.951836
5	1.047660	3.983263	-0.738759
5	-1.291099	-2.131010	-3.191473
5	-2.651564	-1.066157	-2.977910
5	-2.282080	3.661868	-0.114923
5	2.998422	-2.804559	-1.094257
5	-1.461666	-3.346188	-1.984673
5	4.034754	-0.951973	0.757958
5	2.145441	-0.441836	-3.637393
5	4.175250	0.681336	0.612083
5	4.229698	0.929828	-1.039119
5	-4.221797	-0.951566	1.016423
5	2.259750	-3.669195	0.150740
5	-4.167274	-0.700161	-0.633795
5	-4.038888	0.937974	-0.773035
5	-1.302782	1.545196	-3.690661
5	-1.020049	-3.968415	0.720205
5	-1.005595	2.920716	-2.686675
5	-2.402524	2.949239	-1.719724
5	1.316836	-1.531695	3.705194
5	-3.049791	2.801675	1.104578
5	-2.108193	0.420697	3.681725
5	2.392813	-2.932760	1.734049
5	0.992255	-2.899642	2.699169
6	0.901245	-0.699098	0.952156
6	-0.907824	0.709412	-0.940138
6	-2.499524	0.668846	-3.041545
6	2.506158	-0.654637	3.040871
6	3.904509	-1.532944	-0.708207
6	-3.931967	1.513980	0.694835
6	3.424686	1.622071	1.672810
6	-3.407420	-1.627862	-1.695106
6	1.679743	-1.342976	1.957378
6	1.050367	-2.863371	-0.921112
6	3.085281	-0.185004	-0.469645

6	1.854123	1.706758	1.633590
6	-0.502356	0.269283	3.085558
6	-1.214464	-2.431953	1.487677
6	-1.218182	2.802394	0.923220
6	1.211657	2.440230	-1.491207
6	0.515179	-0.256256	-3.065630
6	-1.846137	-1.691827	-1.642403
6	-3.095575	0.177228	0.465625
6	-1.679322	1.356481	-1.950746
7	3.161650	-1.612525	1.939819
7	-3.162101	1.619196	-1.938693
7	3.967766	-0.423140	-1.676683
7	-4.000957	0.403736	1.659280
7	2.722408	2.877080	1.126335
7	-2.686811	-2.885674	-1.152103
5	1.506051	-1.953288	-3.251711
5	-1.505668	1.943985	3.281666
7	2.195002	2.132588	-2.625942
6	0.252010	3.508208	-1.931613
5	2.580318	3.229271	-0.452547
5	3.294556	2.263189	-1.679587
7	0.100066	-1.648304	-3.567009
6	0.135516	1.014222	-3.853442
5	1.673117	1.186074	-3.667408
5	-2.548197	-3.256894	0.430675
5	-3.271834	-2.293178	1.655322
7	-2.191386	-2.153824	2.630218
6	-0.252816	-3.495293	1.938410
6	-0.127512	-1.017534	3.853252
7	-0.082539	1.677471	3.548724
5	-1.664145	-1.220439	3.673059
7	-1.980147	2.758179	2.153478
6	0.497065	4.055212	0.869820
5	-0.850224	4.360914	0.419169
6	-0.379593	-3.952946	-0.920393
7	1.918887	-2.784244	-2.118998
5	0.885490	-4.425832	-0.358813

3e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	0.488630	0.862779	-1.338215
5	1.342534	-0.552973	-0.808477
5	-0.467407	-0.904776	1.373955
5	-1.304195	0.533095	0.844748
5	1.294149	-0.747042	0.975711
5	-1.262465	0.679173	-0.908540
5	0.316512	0.675947	1.506526
5	0.258566	-1.648970	-0.095452
5	-0.231386	1.627996	0.114966



5	-0.273713	-0.712852	-1.470284
5	1.430170	-4.526145	0.256576
5	-1.332295	1.188206	-3.459545
5	-2.565011	1.352774	-1.939266
5	-1.378500	4.574833	-0.238225
5	0.136964	1.992468	3.088733
5	0.494226	-1.012508	4.086092
5	-2.668950	2.668602	1.796699
5	2.721371	-2.662319	-1.883210
5	2.651525	2.237458	-1.801335
5	-2.652567	-2.251457	1.803306
6	-1.251556	-0.833283	-0.105028
6	1.277215	0.801668	0.129752
5	1.317419	0.780501	3.057644
5	4.816288	-0.895026	0.638617
5	2.603235	-0.860069	-1.917878
5	-0.454899	3.241001	0.405918
5	0.067708	2.379584	-2.917908
5	-4.777822	0.840258	-0.777847
5	-2.610858	0.854355	1.887616
5	-0.077514	-2.344903	3.160789
5	0.474208	-3.248994	-0.392237
5	-1.383242	-0.728380	-3.094028
5	-2.528396	-1.621669	0.184586
5	2.545060	1.594825	-0.178327
7	2.418713	3.165948	-0.499828
7	-2.406047	-3.182318	0.527833
5	2.679205	-1.519507	1.796248
6	4.719879	0.407712	1.172380
6	-4.760316	-0.491303	-1.212542
6	4.101434	-0.179179	-1.847223
6	-4.120919	0.177644	1.730644
6	1.348430	1.665371	-2.584906
6	-1.356679	-1.685963	2.597073
6	1.207853	3.888496	-0.214097
6	-1.171338	-3.898193	0.266053
6	2.632073	2.356488	1.959853
6	-2.620987	-2.416020	-1.939429
5	3.966440	1.280409	-1.471950
5	4.394613	1.558978	0.168756
6	3.344684	2.595478	0.722756
6	-3.327429	-2.644480	-0.698133
5	-3.968447	-1.290869	1.449732
5	-4.396717	-1.612962	-0.181802
5	3.551151	-0.001237	2.072104
5	3.255552	-2.539625	0.443432
7	4.516404	-2.023947	-0.117930
7	2.715268	1.143047	2.605151
5	1.226745	3.053614	2.222055
5	0.227378	0.456688	4.214553
5	-0.048732	4.240373	-1.118329
5	-2.373656	3.649423	0.513005

7	0.742624	3.849548	1.134158
7	-0.553989	3.538572	-2.385384
5	-1.596417	2.604329	-2.672313
5	1.272414	0.412613	-3.579717
5	1.547890	-1.903022	-3.022267
5	4.165828	-1.633958	-1.526563
7	2.186530	-0.682518	-3.416673
5	-3.577596	-0.098486	-2.096232
7	-4.382412	1.984340	-0.091516
5	-3.138131	2.538235	-0.655130
7	-0.724250	-3.876288	-1.088690
5	0.100091	-4.160696	1.179317
5	2.383427	-3.681360	-0.642548
5	-0.330609	0.049825	-4.093885
5	-0.163616	-1.919505	-2.970883
5	-1.207298	-3.074633	-2.172818
7	-2.730175	-1.217134	-2.595912
7	-2.200646	0.717985	3.376251
5	-4.107988	1.607494	1.332079
5	-1.594761	1.979185	3.018848
5	-1.273312	-0.377256	3.508389
5	1.729302	-2.638272	2.460533
7	0.604472	-3.444996	2.474751

CBN clusters from pentagonal pyramid isomer IV

4a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.038985	1.356430	0.785360
5	1.363086	0.705522	0.224292
5	0.038985	-1.356430	-0.785360
5	-1.363086	-0.705522	-0.224292
5	1.244360	-0.916945	0.266656
5	-1.244360	0.916945	-0.266656
5	-0.241034	-1.267175	0.842407
5	1.036380	-0.124942	-1.169996
5	-1.036380	0.124942	1.169996
5	0.241034	1.267175	-0.842407
5	-3.136068	1.811601	-1.978292
5	0.235113	-2.450506	3.109084
5	3.136068	-1.811601	1.978292
5	-0.235113	2.450506	-3.109084
5	-1.484288	0.144276	3.845104
5	-3.216503	-1.425673	-1.959934
5	3.216503	1.425673	1.959934
5	0.174502	0.101414	4.192267
5	1.207878	1.342033	3.839660

5	-1.207878	-1.342033	-3.839660
6	-0.558927	0.002639	-1.429930
6	0.558927	-0.002639	1.429930
6	2.489736	0.653873	3.175080
6	-2.489736	-0.653873	-3.175080
6	-2.638224	-2.769344	-1.259277
6	2.638224	2.769344	1.259277
6	-3.841561	1.082235	-0.739958
6	3.841561	-1.082235	0.739958
6	0.843714	-3.399886	1.965791
6	-0.843714	3.399886	-1.965791
6	-2.270724	-1.063498	3.176242
6	2.012831	-0.171614	-2.229246
6	0.125604	-2.614441	-1.484338
6	-2.590672	-1.430486	-0.396881
6	-2.424245	1.724660	-0.451756
6	0.431830	2.482372	-1.581551
6	-0.125604	2.614441	1.484338
6	2.590672	1.430486	0.396881
6	2.424245	-1.724660	0.451756
6	-0.431830	-2.482372	1.581551
6	-2.012831	0.171614	2.229246
6	1.070217	0.051707	2.771300
6	-1.070217	-0.051707	-2.771300
5	-2.439412	0.902343	-3.220375
5	-0.174502	-0.101414	-4.192267
7	-0.969979	1.205087	-3.685092
7	0.969979	-1.205087	3.685092
5	2.439412	-0.902343	3.220375
5	3.500842	0.619470	-2.220973
6	2.270724	1.063498	-3.176242
5	-3.500842	-0.619470	2.220973
5	1.423117	-3.686567	-1.434950
5	-1.423117	3.686567	1.434950
5	-3.004763	-2.880394	0.323892
5	3.004763	2.880394	-0.323892
5	-3.691416	1.898276	0.645210
5	3.691416	-1.898276	-0.645210
5	0.293807	4.050877	-1.003855
5	-0.293807	-4.050877	1.003855
7	3.885420	0.616964	0.756366
5	3.838585	1.447035	-0.688903
5	2.666983	-3.200607	-0.284445
7	2.325331	-3.004926	1.331852
7	-1.330940	-2.433280	2.858045
5	-1.776381	-3.427113	1.518999
7	-2.090070	1.439310	3.129470
5	-3.399598	1.074229	2.181680
7	1.175759	3.382500	1.818141
6	-1.087277	2.796366	2.736592
7	1.330940	2.433280	-2.858045
5	1.776381	3.427113	-1.518999

7	-2.325331	3.004926	-1.331852
5	-2.666983	3.200607	0.284445
7	2.090070	-1.439310	-3.129470
5	3.399598	-1.074229	-2.181680
5	1.484288	-0.144276	-3.845104
7	-3.885420	-0.616964	-0.756366
5	-3.838585	-1.447035	0.688903
5	0.477042	2.700646	3.090765
5	-0.477042	-2.700646	-3.090765
7	-1.175759	-3.382500	-1.818141
5	-0.072509	-4.092439	-0.764783
6	1.087277	-2.796366	-2.736592
5	0.072509	4.092439	0.764783

4b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.072799	1.397605	0.754654
5	1.361898	0.793263	0.172543
5	0.072799	-1.397605	-0.754654
5	-1.361898	-0.793263	-0.172543
5	1.267688	-0.890654	0.254825
5	-1.267688	0.890654	-0.254825
5	-0.213393	-1.380460	0.901257
5	1.030947	-0.077428	-1.177264
5	-1.030947	0.077428	1.177264
5	0.213393	1.380460	-0.901257
5	-2.449457	3.089308	-1.408703
5	-2.176791	1.503129	3.176184
5	2.449457	-3.089308	1.408703
5	-1.272253	-3.612758	-1.882414
5	-4.066145	-0.654770	-0.650047
5	1.606917	2.798380	-2.746112
5	4.066145	0.654770	0.650047
5	0.182060	0.217899	3.988577
5	1.101941	1.559915	3.556134
5	-1.606917	-2.798380	2.746112
5	1.272253	3.612758	1.882414
5	-1.101941	-1.559915	-3.556134
6	-0.556981	-0.015808	-1.359745
6	0.556981	0.015808	1.359745
6	2.527876	0.899084	2.917014
6	-2.527876	-0.899084	-2.917014
6	1.986725	-0.096475	-2.260866
6	0.135366	-2.669904	-1.488901
6	-2.619984	-1.517038	-0.379981
6	-2.455889	1.690781	-0.492223
6	0.479384	2.752070	-1.491281
6	-0.135366	2.669904	1.488901

6	2.619984	1.517038	0.379981
6	2.455889	-1.690781	0.492223
6	-0.479384	-2.752070	1.491281
6	-1.986725	0.096475	2.260866
6	1.126296	0.177748	2.634115
6	-1.126296	-0.177748	-2.634115
5	-2.489426	0.694684	-3.023953
5	-0.182060	-0.217899	-3.988577
7	-1.151184	0.922598	-3.643720
7	1.151184	-0.922598	3.643720
5	2.489426	-0.694684	3.023953
5	2.176791	-1.503129	-3.176184
5	-3.505394	-0.590410	2.139404
5	1.396156	-3.703586	-1.281248
5	-1.396156	3.703586	1.281248
5	-3.144229	-2.878314	0.361944
5	3.144229	2.878314	-0.361944
5	-3.577438	1.920117	0.707726
5	3.577438	-1.920117	-0.707726
5	-0.853534	-3.957508	0.508177
7	1.504848	-0.106840	-3.724325
5	2.330885	1.232312	-3.211904
5	-1.013578	3.408686	-2.299539
7	0.160846	3.314815	-2.912602
7	-3.164374	1.729806	-1.887036
5	-4.005533	1.059665	-0.709561
6	-2.623104	3.149586	0.176259
6	2.020096	3.546752	-1.386578
5	0.853534	3.957508	-0.508177
5	3.505394	0.590410	-2.139404
6	3.306698	-1.023122	-2.163382
6	-3.825366	-1.450306	0.677125
5	-2.801446	-2.977536	-1.281205
7	-3.281331	-1.567763	-1.774566
7	-0.419104	-2.832492	-2.920899
5	1.201222	-2.914345	-2.778966
6	-0.173827	-4.121935	-0.882032
6	0.173827	4.121935	0.882032
7	0.419104	2.832492	2.920899
7	3.281331	1.567763	1.774566
6	3.825366	1.450306	-0.677125
5	2.801446	2.977536	1.281205
5	-1.201222	2.914345	2.778966
6	2.623104	-3.149586	-0.176259
7	3.164374	-1.729806	1.887036
5	4.005533	-1.059665	0.709561
5	1.013578	-3.408686	2.299539
6	-2.020096	-3.546752	1.386578
7	-0.160846	-3.314815	2.912602
7	-1.504848	0.106840	3.724325
6	-3.306698	1.023122	2.163382
5	-2.330885	-1.232312	3.211904

4c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	1.049753	0.780796	-0.856465
5	1.211958	0.578246	0.761514
5	-1.049753	-0.780796	0.856465
5	-1.211958	-0.578246	-0.761514
5	-0.259716	0.550958	1.440422
5	0.259716	-0.550958	-1.440422
5	-1.330642	0.717456	0.232574
5	0.538811	-0.867651	1.183981
5	-0.538811	0.867651	-1.183981
5	1.330642	-0.717456	-0.232574
5	0.435276	-2.675444	-3.195768
5	-2.550668	3.019130	0.737150
5	-0.435276	2.675444	3.195768
5	2.204556	3.173188	-1.622021
5	2.550668	-3.019130	-0.737150
5	-1.142648	3.347999	-2.228517
5	-2.527060	-2.749038	-1.644744
5	-2.204556	-3.173188	1.622021
5	2.527060	2.749038	1.644744
5	-0.397552	4.063421	-0.843666
5	1.221111	4.009522	-0.435015
5	-1.221111	-4.009522	0.435015
6	-0.051604	-1.521014	-0.171231
6	0.051604	1.521014	0.171231
6	1.265252	3.689457	1.148721
6	-1.265252	-3.689457	-1.148721
6	1.113545	-1.678591	2.223789
6	-1.971698	-1.507768	1.689160
6	-2.380786	-1.117313	-1.386437
6	0.421194	-1.067311	-2.774587
6	2.553427	-1.391235	-0.535359
6	1.971698	1.507768	-1.689160
6	2.380786	1.117313	1.386437
6	-0.421194	1.067311	2.774587
6	-2.553427	1.391235	0.535359
6	-1.113545	1.678591	-2.223789
6	0.139702	2.942872	0.291576
6	-0.139702	-2.942872	-0.291576
5	0.156954	-3.690649	-1.827598
5	0.397552	-4.063421	0.843666
7	1.148887	-3.764763	-0.586180
7	-1.148887	3.764763	0.586180
5	-0.156954	3.690649	1.827598
5	1.142648	-3.347999	2.228517
6	-3.721966	0.745821	1.412713

7	-3.237307	2.271135	-0.545819
5	-3.927307	0.856048	-0.177178
5	-2.913285	1.995047	2.043649
5	-2.551032	2.439219	-2.109412
5	-0.936208	1.146910	-3.774648
7	-0.204105	2.443353	-3.222963
6	-2.382499	1.165427	-3.075376
6	2.313363	1.023576	-3.186525
5	3.405347	0.758824	-2.043768
5	1.521053	2.412925	-2.983952
7	3.301006	2.043847	-1.113758
7	2.308028	1.648100	2.848428
7	-1.746524	1.726500	3.221357
5	3.063710	0.264045	2.615565
5	3.565326	1.917906	0.560314
5	-1.473295	0.257581	3.770021
5	0.813187	1.639590	3.689814
6	0.102336	0.243319	4.058165
6	3.831041	0.455657	1.211421
6	3.721966	-0.745821	-1.412713
5	3.927307	-0.856048	0.177178
7	3.237307	-2.271135	0.545819
5	2.913285	-1.995047	-2.043649
5	1.473295	-0.257581	-3.770021
5	-0.813187	-1.639590	-3.689814
6	-0.102336	-0.243319	-4.058165
7	1.746524	-1.726500	-3.221357
7	-2.308028	-1.648100	-2.848428
5	-3.063710	-0.264045	-2.615565
5	-3.565326	-1.917906	-0.560314
6	-3.831041	-0.455657	-1.211421
6	-2.313363	-1.023576	3.186525
5	-3.405347	-0.758824	2.043768
5	-1.521053	-2.412925	2.983952
7	-3.301006	-2.043847	1.113758
7	0.204105	-2.443353	3.222963
6	2.382499	-1.165427	3.075376
5	2.551032	-2.439219	2.109412
5	0.936208	-1.146910	3.774648

4d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.184060	1.522590	-0.151859
5	1.146518	0.739458	-0.720097
5	0.184060	-1.522590	0.151859
5	-1.146518	-0.739458	0.720097
5	1.483127	-0.520294	0.257525
5	-1.483127	0.520294	-0.257525

5	0.310225	-0.492312	1.412657
5	0.713532	-0.763420	-1.183025
5	-0.713532	0.763420	1.183025
5	-0.310225	0.492312	-1.412657
5	-3.988468	0.081982	-1.422396
5	-3.269995	1.483949	-2.040672
5	1.569639	0.007649	3.742728
5	3.269995	-1.483949	2.040672
5	3.988468	-0.081982	1.422396
5	-1.569639	-0.007649	-3.742728
5	-3.225184	-2.493947	0.635131
5	-3.802670	-0.990339	1.183852
5	0.099334	0.124911	-4.026099
5	3.802670	0.990339	-1.183852
5	3.225184	2.493947	-0.635131
5	1.115573	2.659648	2.958505
5	1.573477	3.415618	1.521226
5	-0.099334	-0.124911	4.026099
5	0.719045	3.794077	-1.157297
5	-1.573477	-3.415618	-1.521226
6	-0.881638	-0.877680	-0.857605
6	0.881638	0.877680	0.857605
6	2.878866	2.648111	1.001771
6	-2.878866	-2.648111	-1.001771
6	-2.090579	-3.019983	1.712522
6	2.090579	3.019983	-1.712522
6	-4.119444	0.331481	0.185624
6	4.119444	-0.331481	-0.185624
6	2.053216	-1.450331	3.204101
6	-2.053216	1.450331	-3.204101
6	1.391376	-1.470746	-2.245538
6	0.408955	-2.927630	0.329062
6	-2.203119	-1.461321	1.367544
6	-2.843178	0.924624	-0.550283
6	-0.622816	0.903108	-2.746081
6	-0.408955	2.927630	-0.329062
6	2.203119	1.461321	-1.367544
6	2.843178	-0.924624	0.550283
6	0.622816	-0.903108	2.746081
6	-1.391376	1.470746	2.245538
6	1.679785	1.764534	1.615026
6	-1.679785	-1.764534	-1.615026
5	-3.325477	-1.453407	-1.953690
5	-1.115573	-2.659648	-2.958505
7	-2.124938	-1.423537	-3.049356
7	2.124938	1.423537	3.049356
5	3.325477	1.453407	1.953690
5	2.592917	-0.707773	-3.062266
5	0.562608	-2.456272	-3.314255
5	1.908476	-3.549762	0.632519
5	-1.908476	3.549762	-0.632519
5	-1.877345	-1.980572	2.893309



7	-2.899498	-0.812171	2.610961
7	2.899498	0.812171	-2.610961
5	1.877345	1.980572	-2.893309
5	-3.711437	1.802491	0.614330
7	-3.128978	2.446491	-0.754235
7	3.128978	-2.446491	0.754235
5	3.711437	-1.802491	-0.614330
5	-0.877049	2.495010	-3.032903
7	0.456590	1.635864	-3.586906
7	-0.456590	-1.635864	3.586906
5	0.877049	-2.495010	3.032903
7	0.425423	3.960613	0.435748
5	-2.957914	2.104411	2.165297
6	-0.734089	3.566473	-1.768760
5	-1.165578	3.826588	0.876472
7	-1.173695	1.004877	3.721029
5	-0.562608	2.456272	3.314255
6	-1.633065	3.030897	2.298160
5	-2.592917	0.707773	3.062266
7	-0.425423	-3.960613	-0.435748
6	0.734089	-3.566473	1.768760
5	1.165578	-3.826588	-0.876472
5	-0.719045	-3.794077	1.157297
5	2.957914	-2.104411	-2.165297
7	1.173695	-1.004877	-3.721029
6	1.633065	-3.030897	-2.298160

4f

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	0.901379	-0.977426	-1.385935
5	-0.732281	-1.457529	-0.814912
5	-0.886312	0.558209	1.011812
5	0.692143	1.018406	0.607402
5	-0.962518	-1.058866	0.776836
5	0.580982	-1.742730	0.168014
5	0.966914	0.821373	-1.059942
5	-0.584070	1.293655	-0.464161
5	-1.650656	-0.051110	-0.401589
5	1.652581	-0.306810	0.028986
5	1.321267	3.676729	-1.767166
5	1.959248	-0.374374	-3.444276
5	0.867166	2.668861	-2.977388
5	4.595652	-0.422388	-0.306189
5	-1.590904	-3.626174	1.418829
5	-1.069282	2.323841	3.225263
5	-3.010383	-0.937091	2.530318
5	4.348204	1.154372	0.186008
5	-1.701397	2.214688	-3.076406

5	0.621532	3.697696	1.444806
5	1.415328	0.239518	3.807479
5	2.109727	3.349262	0.820413
5	-1.311842	0.735410	3.808189
5	-2.836944	0.791995	-2.979682
5	-2.157978	-1.893912	-2.975483
5	-3.432558	-2.123654	-1.773080
5	-3.985782	1.823786	-0.738348
5	-0.075738	-0.542475	4.008249
5	-0.522551	-4.036520	0.144308
5	-4.199827	1.010707	0.703202
5	1.553957	-3.465335	-0.958820
5	0.712763	-2.867407	-2.427845
5	-2.059930	3.446077	0.761002
5	-2.863753	3.156402	-0.709296
6	-2.266018	2.634233	2.167977
6	-1.714405	3.358550	-1.855115
6	-3.977332	0.653318	-1.858398
6	-0.900375	-2.984301	-2.621460
6	-0.261545	1.842987	-3.714669
6	2.465533	3.221300	-0.745061
6	0.416851	2.835613	2.780930
6	0.093052	-2.069519	3.273734
6	2.963461	-2.917263	-0.892199
6	-2.924920	-2.857860	0.771301
6	3.590490	1.062548	1.575138
6	3.233491	0.224185	-2.691000
6	0.475542	-0.452117	1.234459
6	-0.413205	0.031573	-1.627040
6	0.805063	-0.716813	2.574445
6	-1.588860	1.165690	2.161088
6	-1.888261	-1.697686	1.752069
6	-3.132379	0.263461	-0.523963
6	-1.243242	2.610742	-0.560587
6	-1.338976	-2.825143	-1.037719
6	0.914270	-3.257387	0.422883
6	1.776029	-1.755491	-2.705580
6	-0.672957	0.171120	-3.055943
6	3.084239	-0.074876	0.423147
6	1.721985	1.899610	-1.822268
6	1.186930	2.095515	1.467874
5	-0.331157	3.932429	-1.186555
7	-0.583395	3.884481	0.372275
7	2.654891	2.179136	1.958256
5	1.623045	1.898098	3.177371
5	3.647171	2.182268	-0.992699
7	3.124960	1.494769	-2.208800
7	3.971466	-1.293757	0.967950
5	3.426587	-0.406120	2.118852
5	4.006877	-0.850886	-1.855240
7	3.158625	-2.020591	-1.936648
7	2.054030	-3.004871	1.486489

5	3.195868	-2.589897	0.620773
5	-0.575381	-4.173173	-1.590411
7	-2.770274	-2.870134	-0.717471
7	-1.157587	-2.734435	2.585163
5	-3.830937	-1.682300	1.291087
5	-4.331772	-0.782263	-1.293129
7	-4.279655	-0.548720	0.285982
7	-2.731185	0.405022	3.052054
5	-3.379286	1.512253	2.134760
5	0.527310	0.486094	-3.953480
7	-1.992843	-0.429018	-3.339108
7	2.312840	-0.941973	3.012754
5	1.605563	-2.345950	2.738769

4g

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.051593	1.347355	0.789728
5	1.351423	0.713402	0.220847
5	0.051593	-1.347355	-0.789728
5	-1.351423	-0.713402	-0.220847
5	1.250101	-0.905057	0.252863
5	-1.250101	0.905057	-0.252863
5	-0.228131	-1.267095	0.822140
5	1.036453	-0.110290	-1.166387
5	-1.036453	0.110290	1.166387
5	0.228131	1.267095	-0.822140
5	-3.276920	1.875519	-1.942392
5	-2.320912	3.123482	-1.339568
5	0.199290	-2.589099	3.132962
5	-2.115954	1.564928	3.168238
5	2.320912	-3.123482	1.339568
5	3.276920	-1.875519	1.942392
5	0.419482	2.844548	3.120238
5	-1.268312	-3.472002	-1.795316
5	-0.199290	2.589099	-3.132962
5	-1.620101	0.113834	3.912725
5	-3.323932	-1.513628	-1.926838
5	-4.008209	-0.555585	-0.702255
5	1.489067	2.457404	-2.883908
5	-0.419482	-2.844548	-3.120238
5	4.008209	0.555585	0.702255
5	3.323932	1.513628	1.926838
5	0.133287	0.038908	4.171372
5	1.130185	1.353438	3.819606
5	-1.489067	-2.457404	2.883908
5	1.268312	3.472002	1.795316
5	-1.130185	-1.353438	-3.819606

6	-0.561337	0.007522	-1.428649
6	0.561337	-0.007522	1.428649
6	2.473231	0.715914	3.152923
6	-2.473231	-0.715914	-3.152923
6	-2.677189	-2.840123	-1.149800
6	2.677189	2.840123	1.149800
6	-3.903040	1.113923	-0.630791
6	3.903040	-1.113923	0.630791
6	0.789358	-3.493793	1.904485
6	-0.789358	3.493793	-1.904485
6	1.172019	-2.870829	-2.682411
6	-1.172019	2.870829	2.682411
6	-2.402553	-1.090716	3.129058
6	1.950000	-0.191668	-2.281359
6	0.067967	-2.575621	-1.548087
6	-2.594401	-1.390306	-0.459158
6	-2.417516	1.704675	-0.540141
6	0.405005	2.440316	-1.618646
6	-0.067967	2.575621	1.548087
6	2.594401	1.390306	0.459158
6	2.417516	-1.704675	0.540141
6	-0.405005	-2.440316	1.618646
6	-1.950000	0.191668	2.281359
6	1.070315	0.035778	2.763901
6	-1.070315	-0.035778	-2.763901
5	-2.500827	0.867022	-3.161506
5	-0.133287	-0.038908	-4.171372
7	-1.009261	1.247461	-3.646906
7	1.009261	-1.247461	3.646906
5	2.500827	-0.867022	3.161506
5	3.389674	0.602934	-2.019477
7	3.279275	-0.984255	-2.043061
5	2.115954	-1.564928	-3.168238
5	1.620101	-0.113834	-3.912725
6	2.402553	1.090716	-3.129058
7	-3.279275	0.984255	2.043061
5	-3.389674	-0.602934	2.019477
7	-0.021794	-3.913369	-0.710277
5	1.417007	-3.505763	-1.271776
7	0.021794	3.913369	0.710277
5	-1.417007	3.505763	1.271776
5	-2.823134	-2.766099	0.409713
7	-3.656118	-1.409819	0.685300
7	3.656118	1.409819	-0.685300
5	2.823134	2.766099	-0.409713
5	-3.498229	1.793405	0.717716
7	-2.566979	3.030001	0.302752
7	2.566979	-3.030001	-0.302752
5	3.498229	-1.793405	-0.717716
5	0.302144	3.872462	-0.841179
7	1.695544	3.281186	-1.444857
7	-1.695544	-3.281186	1.444857

5            -0.302144 -3.872462 0.841179

CBN clusters from pentagonal pyramid isomer V

5a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	0.020411	1.335467	-1.808962
5	0.552143	2.217681	-0.345601
5	0.375056	-0.293236	1.105699
5	-0.276083	-1.085524	-0.303589
5	-0.077678	1.404622	1.093399
5	0.509583	-0.305395	-1.718658
5	-1.145917	0.099737	0.569763
5	1.494398	0.983677	0.616922
5	-1.056963	0.085192	-1.157111
5	1.636387	0.872479	-1.113148
5	1.673226	0.920520	3.452812
5	5.115044	2.452026	-2.045544
5	4.424254	0.472566	-2.740130
5	-1.940996	-1.519209	-3.265586
5	-3.101327	-2.389840	1.004021
5	-1.468639	-2.091657	2.987848
5	-2.139881	-3.266485	-1.290320
5	3.259536	2.934673	2.316382
5	3.472746	-2.485602	-0.462053
5	4.503163	3.444758	0.176301
5	1.879314	-3.220260	1.430481
6	1.254993	-0.612912	-0.216104
6	-1.063561	1.455811	-0.329487
6	-3.523545	2.409071	0.927519
6	1.397267	-3.713119	0.053168
6	2.238328	-3.213496	-1.058781
5	-2.486513	-0.582800	1.146338
5	-0.365277	2.126666	2.595632
5	-0.019868	3.867878	-0.178527
5	-2.301425	-0.545269	-1.854339
5	-0.756848	2.197023	-3.051959
5	0.750364	-1.135611	-3.152067
5	-0.810486	-2.623227	-0.316795
5	0.225085	-1.425563	2.267372
5	2.813827	1.032054	1.638035
5	3.254071	0.482439	-1.376827
5	1.928774	-1.990249	0.033107
5	-2.532018	2.004754	-0.362925
7	-3.956906	1.243399	-1.155810

7	3.056816	-2.336155	1.105857
7	0.240568	1.278675	3.674803
5	-0.845175	0.325458	3.684757
6	-2.672777	2.263058	2.209748
6	1.649370	-2.800344	-2.426046
7	-0.457597	-2.025499	-3.417808
6	-2.022969	4.362815	-0.140114
7	3.946896	3.554624	1.392818
7	-2.205936	-3.326091	0.252309
6	-0.015256	-4.071518	-0.228977
7	5.177390	1.571073	-3.046985
6	-2.632967	2.758899	-2.835819
6	0.860614	-2.956848	2.619947
7	-0.492140	-1.179074	3.674902
7	-2.786279	-2.122070	-2.104220
6	-3.782067	0.068326	-2.119365
6	3.230020	-1.113095	1.956355
7	2.612937	1.925125	2.930484
7	-2.767450	-1.670499	2.300057
6	-4.064070	-0.126578	1.002902
6	4.068767	-1.239801	-1.136540
7	5.025379	3.296818	-1.013797
5	-3.609939	2.645238	-1.616631
5	-3.329243	3.495069	-0.224420
6	-3.999107	1.176248	0.329228
6	-3.736191	-1.206112	-1.419184
5	-2.752110	0.143246	-3.359558
5	2.119638	-0.756503	3.124198
6	3.851875	-0.048332	1.307605
6	-3.422482	-0.279834	2.369517
5	-3.964682	-1.357041	0.118845
5	4.246394	-0.078536	-0.198202
6	3.676512	-0.837325	-2.529199
6	-1.541718	3.095375	2.291164
5	-2.477513	0.830548	2.917114
5	2.326286	-1.539072	-3.095665
6	0.219117	-3.023286	-2.667863
6	-1.057426	4.416499	-1.205302
5	-1.146304	4.089258	1.110818
5	-0.646902	-3.805095	-1.623862
6	-0.947377	-3.801404	0.847019
6	-2.118025	1.605928	-3.501741
5	-1.362304	3.681346	-2.587007
5	-0.586676	-3.259459	2.268267
6	1.044274	-1.804023	3.535117

5b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

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5	-0.233522	1.515718	0.736653
5	1.273976	1.051766	0.012384
5	0.303453	-1.494407	-0.738145
5	-1.235177	-1.017752	-0.065347
5	1.593225	-0.655358	0.287097
5	-1.489229	0.724884	-0.245913
5	0.083360	-1.339722	1.088986
5	1.163426	-0.044633	-1.361433
5	-1.096305	0.046388	1.344485
5	-0.036438	1.349507	-1.139535
5	-1.500062	0.975431	-3.352646
6	-0.547286	-0.251904	-1.440625
6	0.625297	0.261217	1.401215
6	3.082667	-0.307156	3.452281
6	-2.622859	-0.952436	-3.081254
6	-2.981983	0.395200	-3.267459
5	-0.600912	-4.295306	1.091397
5	3.294474	-1.078030	0.527805
5	2.540882	1.923313	0.502963
5	-2.959273	-1.302650	2.714981
5	-1.500203	3.461702	1.857384
5	-3.048749	1.301238	-0.597049
5	-2.508290	-1.887749	-0.593175
5	1.529404	-3.441194	-1.709311
5	2.937501	1.319205	-2.782899
5	0.447317	4.223144	-1.081326
5	-0.995597	-0.649252	-3.061202
5	1.079587	0.626483	2.997995
6	-2.809500	-2.818488	2.567471
5	-3.394180	1.523912	2.279053
5	3.478618	-1.548938	-2.282998
6	2.661988	2.833187	-2.653596
6	1.562326	-3.559414	2.049078
5	-1.850637	-3.910167	2.032295
5	1.675351	3.869860	-2.060751
6	-1.733323	3.459049	-1.924135
6	4.440387	-0.036128	0.246458
5	2.931611	-2.885432	2.014891
5	-3.070052	2.733014	-1.666617
6	-4.414344	0.183155	-0.796731
6	2.677636	3.260206	1.566735
5	4.239935	1.465173	0.645376
5	-4.176897	-1.414592	-0.884954
6	-2.642116	-3.278361	-1.635082
6	-2.959515	2.992583	2.012488
5	1.291647	3.327967	2.071139
5	-1.239371	-3.372660	-2.088913
5	-3.373028	-1.994359	-2.175995
6	-2.864396	-3.494680	-0.250277
7	-3.788281	-2.445186	0.266223
7	1.734039	-4.072617	-0.285847
7	4.911804	-1.257928	-1.916304

5	0.181742	-2.747098	-2.322472
6	2.966511	-2.927120	-1.750927
6	2.948503	-3.251715	-0.396700
6	3.543304	2.273464	-1.787658
5	2.396144	-0.253664	-2.773776
5	-0.867808	2.272206	-2.399765
6	-1.140324	4.051993	-0.764664
7	1.863129	4.147956	-0.654717
7	-3.557389	2.721703	-0.346304
6	-4.709393	0.692825	0.457989
5	-3.802585	0.987449	-2.135173
5	3.228893	-1.656334	3.113179
6	4.860492	-0.590446	-0.895083
7	3.497037	-2.592159	0.671367
7	-1.983270	-4.138857	0.618761
6	0.996232	-4.098555	0.842806
5	0.817776	-2.284525	2.365206
5	-2.340646	0.235151	2.774579
6	-3.599777	-2.178384	1.664587
7	-4.689382	1.057498	1.600969
7	-1.792281	4.162720	0.453612
6	-2.978227	3.385828	0.684187
5	-0.128576	2.708997	2.330735
5	3.461886	1.945984	2.023559
6	2.817566	3.542518	0.173519
7	3.754999	2.553131	-0.399975
7	0.076500	-1.704322	-3.490925
5	1.205069	-0.985555	-3.541998
6	2.701618	0.947346	3.009690
7	0.009516	1.635840	3.489346
5	1.518792	-1.005802	3.313437
5	-1.135303	0.941262	3.545951

5c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	1.646583	-0.264571	-0.020401
5	0.956804	1.367888	-0.217634
5	-1.646583	0.264571	0.020401
5	-0.956804	-1.367888	0.217634
5	-0.561522	1.058682	-1.027623
5	0.561522	-1.058682	1.027623
5	-0.812436	-0.584885	-1.271339
5	-0.541271	1.388776	0.666279
5	0.541271	-1.388776	-0.666279
5	0.812436	0.584885	1.271339
5	0.000213	3.877091	0.374915
5	3.799821	-0.588102	1.500024
5	2.285989	-3.133293	0.888724



5	-0.000213	-3.877091	-0.374915
5	-3.312554	-1.034200	-1.486938
5	-3.799821	0.588102	-1.500024
5	-1.587203	-3.714274	-0.950017
5	1.587203	3.714274	0.950017
5	3.312554	1.034200	1.486938
5	-2.839770	0.078513	3.509710
6	-0.739338	-0.104438	1.364539
6	0.739338	0.104438	-1.364539
6	0.837919	1.359353	-4.010565
6	-0.837919	-1.359353	4.010565
5	-1.764101	-1.086765	-2.486516
5	-1.161788	2.152406	-1.998974
5	1.331829	3.108728	-0.509982
5	0.963733	-2.754436	-1.441276
5	3.389442	-0.084941	0.046568
5	1.161788	-2.152406	1.998974
5	-1.331829	-3.108728	0.509982
5	-3.389442	0.084941	-0.046568
5	-0.963733	2.754436	1.441276
5	1.764101	1.086765	2.486516
5	-1.291896	-0.294432	2.782714
5	1.291896	0.294432	-2.782714
7	1.565253	-0.893055	-3.871515
7	-1.565253	0.893055	3.871515
5	-2.285989	3.133293	-0.888724
6	-0.210872	2.296149	-3.518825
6	0.210872	-2.296149	3.518825
6	2.542169	2.369349	-2.368431
6	-2.542169	-2.369349	2.368431
6	3.501666	-0.552926	-2.206071
6	-3.501666	0.552926	2.206071
6	1.296933	-2.183998	-3.272264
6	-1.296933	2.183998	3.272264
6	-0.921121	-0.482544	-4.060892
6	0.921121	0.482544	4.060892
5	2.839770	-0.078513	-3.509710
5	2.315954	1.471483	-3.603206
6	0.433320	-0.020025	-4.206099
6	-0.027970	-2.668215	-3.173868
6	0.027970	2.668215	3.173868
6	-1.914315	0.462658	-3.684366
6	1.914315	-0.462658	3.684366
6	0.134446	3.289133	-2.520975
6	-0.134446	-3.289133	2.520975
6	3.262466	1.849962	-1.280975
6	-3.262466	-1.849962	1.280975
6	3.192949	-1.801581	-1.619046
6	-3.192949	1.801581	1.619046
7	-1.488195	-3.245751	1.965858
5	-2.735287	-2.218241	-0.199507
5	-3.136951	1.910775	0.021853

7	-3.780810	-0.479033	1.267174
7	-2.217350	2.672090	2.314112
5	0.438004	3.678138	2.014282
5	3.152626	-0.009613	2.804296
7	1.171575	1.844302	3.657883
7	1.573185	-1.889465	3.479011
5	0.928021	-3.810025	1.380567
5	2.735287	2.218241	0.199507
7	1.488195	3.245751	-1.965858
7	-1.573185	1.889465	-3.479011
5	-0.928021	3.810025	-1.380567
5	-3.152626	0.009613	-2.804296
7	-1.171575	-1.844302	-3.657883
7	2.217350	-2.672090	-2.314112
5	-0.438004	-3.678138	-2.014282
5	3.136951	-1.910775	-0.021853
7	3.780810	0.479033	-1.267174
6	-0.433320	0.020025	4.206099
5	-2.315954	-1.471483	3.603206

5e

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.141612	1.241528	0.871599
5	1.241580	0.772512	0.178493
5	0.141612	-1.241528	-0.871599
5	-1.241580	-0.772512	-0.178493
5	1.287179	-0.807335	0.140009
5	-1.287179	0.807335	-0.140009
5	-0.088405	-1.318139	0.836593
5	1.066611	0.073204	-1.364549
5	-1.066611	-0.073204	1.364549
5	0.088405	1.318139	-0.836593
5	-3.282472	1.805230	-2.021335
5	0.910945	-2.751693	3.219694
5	3.282472	-1.805230	2.021335
5	0.392834	2.815363	3.068052
5	-0.910945	2.751693	-3.219694
5	-1.215607	-0.226750	3.934462
5	-3.296254	-1.428186	-1.987432
5	-0.392834	-2.815363	-3.068052
5	3.296254	1.428186	1.987432
5	1.215607	0.226750	-3.934462
5	0.440597	-0.144969	4.284400
5	1.251247	1.295036	3.830900
5	-1.251247	-1.295036	-3.830900

5	-0.440597	0.144969	-4.284400
6	-0.592405	0.028612	-1.394858
6	0.592405	-0.028612	1.394858
6	2.583365	-0.937398	3.166917
6	-2.947984	-2.757477	0.257637
6	2.947984	2.757477	-0.257637
6	-3.579725	1.949066	0.533925
6	3.579725	-1.949066	-0.533925
6	-0.466029	-3.846766	0.851558
6	0.466029	3.846766	-0.851558
6	1.400057	-3.649596	-1.142881
6	-1.400057	3.649596	1.142881
6	-3.234414	-0.311535	1.745850
6	3.234414	0.311535	-1.745850
5	0.154025	-2.587642	-1.497599
5	-2.524438	-1.425019	-0.499518
5	-2.411573	1.700961	-0.564305
5	0.256551	2.482984	-1.842726
5	2.041437	-1.070777	-3.707621
5	-0.154025	2.587642	1.497599
5	2.524438	1.425019	0.499518
5	2.411573	-1.700961	0.564305
5	-0.256551	-2.482984	1.842726
5	-2.041437	1.070777	3.707621
5	1.224073	-0.066393	2.748639
5	-1.224073	0.066393	-2.748639
7	-1.081888	-3.518785	-1.752067
5	1.391538	-3.025466	-2.573434
6	-0.042745	-3.885388	-0.611803
6	-3.647837	-1.270880	0.583495
7	-3.915335	-0.633375	-0.745655
5	-2.617717	-2.897248	-1.293919
7	-2.600805	-0.619707	-3.126081
6	-2.583365	0.937398	-3.166917
6	-1.361800	1.367085	-3.823095
7	2.600805	0.619707	3.126081
6	1.361800	-1.367085	3.823095
7	1.081888	3.518785	1.752067
5	-1.391538	3.025466	2.573434
6	0.042745	3.885388	0.611803
7	3.915335	0.633375	0.745655
5	2.617717	2.897248	1.293919
6	3.647837	1.270880	-0.583495
7	-2.395703	3.081378	-1.294805
5	-3.980543	1.076959	-0.747316
6	-2.590987	3.097400	0.198968
6	2.590987	-3.097400	-0.198968
5	3.980543	-1.076959	0.747316
7	2.395703	-3.081378	1.294805
7	1.684573	2.536526	-2.411603
5	-0.918368	3.692916	-1.923049
6	1.827335	3.215570	-1.240198

6	-1.827335	-3.215570	1.240198
5	0.918368	-3.692916	1.923049
7	-1.684573	-2.536526	2.411603
7	2.565839	-1.880674	-2.761087
5	2.114249	1.009698	-2.680148
6	3.313578	-1.156091	-1.750959
6	-3.313578	1.156091	1.750959
5	-2.114249	-1.009698	2.680148
7	-2.565839	1.880674	2.761087

CBN clusters from pentagonal pyramid isomer VI

6a

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.104623	1.291748	0.784732
5	1.273783	0.767070	0.230001
5	0.104623	-1.291748	-0.784732
5	-1.273783	-0.767070	-0.230001
5	1.242900	-0.814227	0.238703
5	-1.242900	0.814227	-0.238703
5	-0.156095	-1.277787	0.798792
5	0.985101	-0.023869	-1.122920
5	-0.985101	0.023869	1.122920
5	0.156095	1.277787	-0.798792
5	1.025820	-1.322717	3.840683
5	1.163126	1.348163	3.792352
5	-1.025820	1.322717	-3.840683
5	-1.163126	-1.348163	-3.792352
6	-0.548422	0.003206	-1.380226
6	0.548422	-0.003206	1.380226
6	2.399440	-0.851517	3.233559
6	2.481244	0.716165	3.201735
6	-2.481244	-0.716165	-3.201735
6	-2.399440	0.851517	-3.233559
5	-0.377081	-2.481978	1.616112
5	2.402455	-1.677864	0.491495
5	2.560765	1.439779	0.438508
5	-1.943694	0.140599	2.221627
5	-0.122692	2.568282	1.518488
5	-2.402455	1.677864	-0.491495
5	-2.560765	-1.439779	-0.438508
5	0.122692	-2.568282	-1.518488
5	1.943694	-0.140599	-2.221627
5	0.377081	2.481978	-1.616112
5	-1.119445	0.007700	-2.724707
5	1.119445	-0.007700	2.724707
7	0.221515	0.064502	4.030697

7	-0.221515	-0.064502	-4.030697
6	2.311986	-3.029637	1.344450
6	-2.311986	3.029637	-1.344450
6	3.913155	0.634775	0.707099
6	-3.913155	-0.634775	-0.707099
6	1.169769	3.454899	1.788021
6	-1.169769	-3.454899	-1.788021
6	-2.062739	1.475367	3.105309
6	2.062739	-1.475367	-3.105309
6	-1.420641	-2.555413	2.811526
6	1.420641	2.555413	-2.811526
7	-2.223793	-1.101748	3.145897
5	-1.327474	0.192638	3.766591
5	-3.432190	-0.568513	2.084048
6	-3.266243	1.041350	2.161977
6	0.091592	3.993526	0.782792
5	0.489755	2.777780	3.072337
5	-1.407569	3.608538	1.248735
7	-1.146556	2.803266	2.673134
7	2.623339	2.813661	1.196209
6	3.737608	1.421880	-0.658503
5	3.275066	1.422358	1.956128
5	2.914525	2.803029	-0.440643
5	3.045546	-1.767356	2.039895
5	3.528188	-1.879600	-0.713535
7	3.815354	-1.038970	0.710772
6	2.612908	-3.110808	-0.204560
6	-1.742662	-3.349900	1.496576
5	0.120860	-2.666236	3.213069
5	-0.393257	-3.969073	0.849014
7	0.779336	-3.492628	1.895959
7	2.223793	1.101748	-3.145897
6	3.266243	-1.041350	-2.161977
5	3.432190	0.568513	-2.084048
5	1.327474	-0.192638	-3.766591
5	0.393257	3.969073	-0.849014
6	1.742662	3.349900	-1.496576
5	-0.120860	2.666236	-3.213069
7	-0.779336	3.492628	-1.895959
7	-3.815354	1.038970	-0.710772
5	-3.045546	1.767356	-2.039895
5	-3.528188	1.879600	0.713535
6	-2.612908	3.110808	0.204560
6	-3.737608	-1.421880	0.658503
5	-2.914525	-2.803029	0.440643
5	-3.275066	-1.422358	-1.956128
7	-2.623339	-2.813661	-1.196209
7	1.146556	-2.803266	-2.673134
5	1.407569	-3.608538	-1.248735
5	-0.489755	-2.777780	-3.072337
6	-0.091592	-3.993526	-0.782792

6c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.081923	1.311632	0.765200
5	1.295236	0.746512	0.209394
5	0.081923	-1.311632	-0.765200
5	-1.295236	-0.746512	-0.209394
5	1.227624	-0.845775	0.232648
5	-1.227624	0.845775	-0.232648
5	-0.190849	-1.276926	0.802935
5	0.995775	-0.057406	-1.118583
5	-0.995775	0.057406	1.118583
5	0.190849	1.276926	-0.802935
5	3.298633	-1.103363	-2.041150
5	0.115902	3.999386	0.661746
5	-2.520866	3.149426	0.290592
5	-3.298633	1.103363	2.041150
5	-1.832434	-3.324109	1.414595
5	-0.115902	-3.999386	-0.661746
5	-3.722851	-1.372623	0.767157
5	3.722851	1.372623	-0.767157
5	0.930906	-1.369757	3.664006
5	1.117178	1.414051	3.598227
5	-0.930906	1.369757	-3.664006
5	1.832434	3.324109	-1.414595
5	-1.117178	-1.414051	-3.598227
6	-0.529368	0.002336	-1.334510
6	0.529368	-0.002336	1.334510
6	2.349054	-0.892961	3.067627
6	2.457756	0.723512	3.030455
6	-2.457756	-0.723512	-3.030455
6	-2.349054	0.892961	-3.067627
5	-0.401087	-2.485726	1.624102
5	2.400455	-1.691322	0.489303
5	2.573719	1.436951	0.427140
5	-1.955054	0.157473	2.220735
5	-0.099068	2.582710	1.515324
5	-2.400455	1.691322	-0.489303
5	-2.573719	-1.436951	-0.427140
5	0.099068	-2.582710	-1.515324
5	1.955054	-0.157473	-2.220735
5	0.401087	2.485726	-1.624102
5	-1.076984	0.004656	-2.649713
5	1.076984	-0.004656	2.649713
7	0.148343	0.088541	3.914931
7	-0.148343	-0.088541	-3.914931
7	3.509139	-1.869934	-0.626401
5	3.887503	-0.977937	0.763443
5	2.520866	-3.149426	-0.290592

6	2.352536	-3.077710	1.301748
6	3.099721	-1.770794	1.906668
6	-3.099721	1.770794	-1.906668
6	-2.352536	3.077710	-1.301748
7	-3.509139	1.869934	0.626401
5	-3.887503	0.977937	-0.763443
5	2.618465	2.876198	1.286768
6	3.968914	0.678757	0.657061
6	3.272309	1.513091	1.844345
7	2.923054	2.755419	-0.369512
7	-2.923054	-2.755419	0.369512
6	-3.272309	-1.513091	-1.844345
6	-3.968914	-0.678757	-0.657061
5	-2.618465	-2.876198	-1.286768
7	-1.336337	3.573102	1.304603
5	-1.169113	2.795137	2.774323
6	1.162650	3.534979	1.772796
6	0.411213	2.812147	2.996948
6	-0.411213	-2.812147	-2.996948
6	-1.162650	-3.534979	-1.772796
7	1.336337	-3.573102	-1.304603
5	1.169113	-2.795137	-2.774323
5	-2.214764	-1.189779	3.190538
7	-3.361658	-0.550082	2.136547
6	-2.153506	1.481674	3.107716
6	-1.490613	0.150070	3.724186
6	1.490613	-0.150070	-3.724186
6	2.153506	-1.481674	-3.107716
5	2.214764	1.189779	-3.190538
7	3.361658	0.550082	-2.136547
7	-0.386335	-3.913117	0.912433
5	0.872220	-3.517639	1.952605
6	-1.470430	-2.622680	2.804425
6	0.106910	-2.719506	3.105189
6	-0.106910	2.719506	-3.105189
6	1.470430	2.622680	-2.804425
5	-0.872220	3.517639	-1.952605
7	0.386335	3.913117	-0.912433

CBN clusters from pentagonal pyramid isomer VII

7b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-1.288556	-0.151942	-1.085303
5	-1.162081	1.186783	-0.003622
5	1.290145	0.223460	0.914936
5	1.226047	-1.150034	-0.124701

5	-0.304336	0.717937	1.479011
5	0.304678	-0.733285	-1.529791
5	0.108514	-0.967582	1.251659
5	0.488851	1.539482	0.224408
5	-0.498791	-1.522950	-0.225730
5	-0.034457	0.955757	-1.414376
5	2.651964	2.108189	-2.650983
5	3.985871	1.668870	-0.524776
6	1.339673	0.400574	-0.720089
6	-1.310588	-0.344083	0.617246
6	4.183588	0.472768	-1.496792
6	3.339422	0.685145	-2.767380
5	0.266177	-1.901491	2.613661
5	-0.871760	1.270284	3.032942
5	-2.409020	2.248728	0.058128
5	-0.901639	-3.101739	-0.051607
5	-2.582722	0.060209	-2.194496
5	0.850419	-1.756185	-2.936975
5	2.504156	-2.251347	-0.131962
5	2.670899	0.123070	1.748019
5	0.978581	3.007060	0.575599
5	-0.769171	2.205922	-3.042764
5	2.614389	0.935140	-1.339168
5	-2.686231	-0.662465	1.209705
7	-3.422634	-2.076682	1.142053
7	3.057849	2.589162	-1.267017
6	-3.144964	-1.529234	2.534550
6	-4.086207	-1.012952	0.361907
5	-3.651715	-0.073763	2.689353
5	-4.204099	0.297916	1.147409
5	-0.186130	-3.811629	1.641485
5	-2.421129	-3.186077	-1.313256
5	-3.902932	1.123722	-1.301784
5	-2.302836	3.188616	1.726280
5	-0.096135	0.058474	3.925290
5	-0.009151	-0.475088	-3.452757
5	2.069279	-3.054999	-2.063868
5	3.923662	-1.189851	1.571902
5	2.800128	2.925145	1.362041
5	0.019690	3.622920	-1.968680
7	-2.496415	-1.279579	-2.996623
6	-3.204026	-2.013492	-1.983030
6	-2.969029	1.590968	-2.384558
5	-3.876226	-0.914649	-1.179348
5	4.356041	0.456962	1.601544
6	3.840887	1.736673	1.084178
7	2.459708	-0.270567	3.180158
6	2.740958	-1.555216	2.570110
6	-0.997031	-3.492857	-2.029358
6	-1.529088	-3.861954	1.294079
7	-0.090700	-3.942104	-1.090795
5	-2.629025	-3.301289	0.443714



5	2.283275	3.574869	-0.331932
6	0.866763	4.085751	-0.711622
6	2.219605	2.578349	2.716667
7	0.035248	4.159873	0.563683
7	1.703071	-2.530100	2.520695
6	1.312300	-3.496977	1.521554
6	-0.597763	-1.409663	3.832334
5	-1.884254	-1.744793	3.356985
5	0.993064	2.290810	-2.981810
6	0.092304	1.074781	-3.268459
6	-1.500630	3.599793	-1.779761
7	-2.076561	2.615767	-2.662391
7	1.742100	1.814076	3.532690
6	1.454621	0.466913	3.759701
6	-2.000965	2.294011	2.990977
5	-2.901631	1.245709	3.341317
5	2.857782	-0.725479	-3.230139
6	2.488920	-2.066916	-3.000024
6	-1.266370	-1.518617	-3.413750
7	-0.518746	-2.675047	-3.079077
7	-2.065160	3.660360	-0.546400
6	-1.347534	3.888568	0.631339
6	-4.121465	1.625296	0.157066
5	-3.753978	2.747592	1.014866
5	4.401582	-0.873879	-0.837300
6	3.992088	-1.793574	0.117255
6	1.311590	-3.801613	-1.004069
7	1.925344	-3.605186	0.296443

7c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-1.358622	0.979119	-0.805025
5	-1.055535	-0.616088	-1.534903
5	0.973662	-1.088663	0.311558
5	0.726477	0.484903	1.003497
5	0.619506	-0.975629	-1.379394
5	-0.955514	0.838627	0.863115
5	1.481234	0.349834	-0.529643
5	-0.524313	-1.743423	-0.338899
5	0.219109	1.582142	-0.279775
5	-1.781240	-0.494386	0.089094
6	-0.419645	-0.767653	1.036855
6	0.144124	0.597888	-1.632644
5	3.178955	0.599350	-0.677472
5	1.662082	-1.637425	-2.469200
5	-1.801016	-0.999574	-2.993489
5	0.645139	3.218677	-0.408234

5	-2.804548	1.887197	-0.968837
5	-1.623786	1.551530	2.206753
5	1.546729	0.787605	2.390478
5	2.148494	-2.002134	0.930962
5	-0.857112	-3.489399	0.015663
5	-3.250597	-0.977495	0.859000
5	-0.680147	-1.447170	2.356445
5	0.460007	1.023785	-3.151056
7	1.961799	2.851027	-2.403047
7	-1.677072	-2.505130	2.511354
6	2.841483	1.876274	-2.539868
6	-1.559991	2.879197	-3.012617
5	2.187832	0.601621	-3.247566
5	-1.215774	1.408607	-3.535699
6	-1.660026	4.199517	-0.822182
6	1.684681	-3.703221	1.021921
6	2.725987	3.206813	-0.050398
6	-3.048236	-3.113022	0.384610
6	4.066152	-1.057388	-0.944509
6	-3.799744	0.534747	2.196206
6	-0.093937	-3.077796	-3.350415
6	-0.215422	2.168173	3.461598
6	-3.474839	0.196397	-2.855337
6	3.053677	-0.322485	2.626538
7	-2.217050	0.350170	-3.551543
6	-1.219240	-2.469548	-3.406255
5	-2.535147	-2.621465	-2.480872
5	-3.692511	-1.291662	-2.545430
5	2.649148	-2.976525	-1.880279
5	1.181259	-3.344897	-2.678215
6	3.383982	-1.605790	-2.122959
7	2.655559	-0.783986	-3.110522
7	3.835979	1.637354	-1.605868
6	3.789026	2.218629	-0.276423
5	4.354725	1.229295	0.732133
5	4.789619	-0.069215	-0.215644
5	1.880916	3.471623	1.245590
5	0.200589	3.997388	1.300892
6	-0.467232	4.211878	-0.105959
7	1.948359	3.486916	-1.138519
7	-1.521178	3.684279	-2.154087
6	-3.855169	1.181407	-1.846264
5	-4.526416	1.382577	-0.599785
5	-2.532259	3.292595	0.058704
5	2.877302	-3.316088	0.049743
5	3.817180	-1.966597	0.412090
7	1.406437	-3.468972	2.377762
6	3.291269	-1.420349	1.727196
6	0.617386	-4.031289	0.049422
7	-1.995582	-3.191046	1.273297
5	-2.208821	-3.463987	-0.958050
5	1.450604	-4.017122	-1.209090

5	-4.396717	1.271554	1.020343
5	-4.280833	-1.816732	-1.146761
7	-3.253746	-0.713196	2.359610
6	-4.074825	-2.135546	0.240375
6	-3.434515	1.872580	2.076787
7	-1.051418	1.031961	3.486266
5	-0.817243	3.254808	2.469102
5	-2.411561	3.038949	1.775031
5	3.534731	1.115343	2.227445
5	2.418709	2.399201	2.623989
7	1.772086	-0.368967	3.310075
6	1.184854	2.165164	3.308823
6	-2.186804	-1.236147	3.077499
6	1.023639	-2.792160	3.283862
5	-0.957236	-0.441117	3.729700
5	0.697137	-1.275633	3.634267

7d

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	0.706304	-1.062279	0.765620
5	1.011881	0.610714	1.187832
5	-0.639601	1.506518	-0.915877
5	-0.905501	-0.203877	-1.263570
5	0.940122	1.728811	-0.196456
5	-0.851312	-1.281190	0.122996
5	0.655944	0.573237	-1.561605
5	-0.464083	1.552729	0.836101
5	0.493483	-1.054181	-0.978420
5	-0.565559	-0.117855	1.445419
5	-2.658359	4.392476	0.188429
5	1.788422	-1.835572	3.225524
5	-2.021615	-2.649062	1.988691
5	0.822790	-4.051596	1.855660
5	2.660157	-2.931330	-0.865225
5	2.779991	3.054394	-1.906938
5	-3.286583	0.712291	-2.608486
5	-1.001468	3.865304	-1.751379
5	1.087265	-3.746051	-0.971902
5	-0.622085	-0.871196	-4.209394
5	-2.501523	-2.912328	-1.431253
5	-1.803176	1.418666	-3.202087
5	-1.068376	-3.208265	-2.461243
5	-2.227596	0.615209	3.189007
5	1.656535	2.805660	2.835743
5	3.019823	2.607329	1.741071
5	-3.595935	3.007332	0.492863
5	4.337830	-0.873627	-1.377979
5	4.610282	-0.773639	0.257570

5	2.301561	-0.182608	-3.355430
5	3.224408	-1.119673	2.542850
5	0.713391	0.638202	4.293922
5	-4.632494	0.310044	-0.372998
5	-4.464014	0.617379	1.273550
6	-1.539642	0.379441	0.130240
6	1.603405	-0.082500	-0.238337
6	4.448183	0.758669	0.610216
6	-4.188941	-1.174654	-0.557655
6	-0.501855	-1.991867	-3.313693
6	0.865086	2.091372	3.925920
6	0.329787	-3.693004	0.489376
6	-1.854575	4.685914	-0.909603
6	-0.730169	0.558767	-3.893388
6	0.797090	-0.633580	3.702861
6	-1.318186	2.485660	-2.091573
6	1.371916	-3.210739	2.812619
6	0.069624	-4.006986	-1.968094
6	0.128754	2.810859	3.003603
5	-1.555259	-0.593454	-2.713378
5	-1.140339	-3.000535	0.580366
5	-0.865785	-0.459689	3.108995
5	-1.129370	2.325773	2.207455
5	-2.576179	3.294701	-1.347633
5	1.816166	0.354853	2.648786
5	1.921777	3.098006	-0.496126
5	0.822882	0.620697	-3.282662
5	0.896123	-1.852512	-2.411686
5	1.416874	-2.522895	1.299067
5	2.923379	-0.999840	-0.280883
5	-3.044861	0.751857	0.268505
6	-4.001711	-0.744526	1.797992
7	-4.009512	-1.786681	0.746539
7	4.297528	1.478441	-0.632933
6	4.180193	0.624354	-1.791006
7	-2.568035	-3.494365	-0.099623
6	-3.196208	-2.852634	0.933260
6	3.708113	2.712711	-0.680660
7	3.092164	3.261110	0.449112
7	-2.022318	-1.643072	3.002252
6	-3.033911	-0.725015	2.814157
6	3.307295	0.958444	-2.846486
7	2.630000	2.142834	-2.949396
7	-2.504826	1.893337	2.568819
6	-3.528850	1.855858	1.513411
6	3.266840	-1.881939	-1.849878
7	2.305905	-1.553291	-2.868573
7	-3.787896	2.648505	-0.945474
6	-4.006098	1.272955	-1.351173
6	3.758314	-1.631628	1.163431
7	2.833518	-2.525503	0.537574
7	-3.093662	-0.722702	-2.656957

6	-3.426499	-1.641328	-1.634986
6	3.805596	1.263664	1.747166
7	3.282434	0.312214	2.695323

CBN clusters from pentagonal pyramid isomer VIII

8b

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
5	-0.348176	1.254085	0.914765
5	1.188187	1.015724	0.308574
5	0.348176	-1.254085	-0.914765
5	-1.188187	-1.015724	-0.308574
5	1.446402	-0.634086	0.196812
5	-1.446402	0.634086	-0.196812
5	0.069516	-1.414030	0.729828
5	1.036324	0.246313	-1.173630
5	-1.036324	-0.246313	1.173630
5	-0.069516	1.414030	-0.729828
5	1.132590	1.293131	3.847592
5	-1.132590	-1.293131	-3.847592
6	-0.538509	0.010179	-1.367110
6	0.538509	-0.010179	1.367110
6	2.450201	0.735875	3.272021
6	-2.450201	-0.735875	-3.272021
5	-0.024981	-2.677257	1.673968
5	2.744873	-1.435463	0.605554
5	2.520714	1.794198	0.657423
5	-1.955901	-0.212329	2.450712
5	-0.363477	2.522527	1.853986
5	-2.744873	1.435463	-0.605554
5	-2.520714	-1.794198	-0.657423
5	0.363477	-2.522527	-1.853986
5	1.955901	0.212329	-2.450712
5	0.024981	2.677257	-1.673968
5	-1.120198	0.032527	-2.719115
5	1.120198	-0.032527	2.719115
7	0.275400	0.021833	4.061756
7	-0.275400	-0.021833	-4.061756
6	3.234097	-1.657792	2.198642
6	-3.234097	1.657792	-2.198642
6	3.189550	1.505563	2.209735
6	-3.189550	-1.505563	-2.209735
6	0.456828	2.599473	3.313385
6	-0.456828	-2.599473	-3.313385
6	-1.217137	0.046021	3.927067
6	1.217137	-0.046021	-3.927067

6	0.390155	-2.486236	3.303511
6	-0.390155	2.486236	-3.303511
5	2.509281	-0.829719	3.344577
6	1.080522	-1.246301	3.772815
6	-1.080522	1.246301	-3.772815
5	-2.509281	0.829719	-3.344577
7	-1.022762	2.646671	3.198918
5	1.283304	3.298303	2.185580
6	0.313419	3.904794	0.914671
5	-1.136791	3.641313	0.555557
7	1.022762	-2.646671	-3.198918
5	1.136791	-3.641313	-0.555557
5	-1.283304	-3.298303	-2.185580
6	-0.313419	-3.904794	-0.914671
7	2.687585	2.803162	1.797610
5	3.925696	0.638974	1.099208
6	3.788395	1.274743	-0.474975
5	2.846746	2.356770	-1.032001
7	-2.687585	-2.803162	-1.797610
5	-2.846746	-2.356770	1.032001
5	-3.925696	-0.638974	-1.099208
6	-3.788395	-1.274743	0.474975
7	4.011351	-0.886162	1.198729
5	2.439877	-2.897490	1.686931
5	2.980874	-2.176632	-1.108297
6	2.520476	-3.129456	-0.022312
7	-4.011351	0.886162	-1.198729
5	-2.980874	2.176632	1.108297
5	-2.439877	2.897490	-1.686931
6	-2.520476	3.129456	0.022312
7	1.142717	-3.343483	2.378964
5	-1.156584	-2.435586	3.125956
5	-1.012270	-3.656590	0.476230
6	-1.736698	-3.203202	1.745860
7	-1.142717	3.343483	-2.378964
5	1.012270	3.656590	-0.476230
5	1.156584	2.435586	-3.125956
6	1.736698	3.203202	-1.745860
7	-1.894660	-1.188215	3.610861
5	-1.844920	1.389442	3.390837
5	-3.535961	-0.116795	1.494609
6	-3.126232	1.131838	2.274780
7	1.894660	1.188215	-3.610861
5	3.535961	0.116795	-1.494609
5	1.844920	-1.389442	-3.390837
6	3.126232	-1.131838	-2.274780

8c

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

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5	-0.420357	1.201055	0.987475
5	1.134395	1.139201	0.274639
5	0.420357	-1.201055	-0.987475
5	-1.134395	-1.139201	-0.274639
5	1.613619	-0.516764	0.191525
5	-1.613619	0.516764	-0.191525
5	0.211777	-1.474735	0.664459
5	1.019369	0.396722	-1.265572
5	-1.019369	-0.396722	1.265572
5	-0.211777	1.474735	-0.664459
5	2.560045	-2.266309	-2.424858
5	-2.896959	1.577761	-2.019239
5	0.434245	4.004184	0.624736
5	-2.193052	3.104459	0.161497
5	0.275300	-2.682164	3.304735
5	2.896959	-1.577761	2.019239
5	0.595519	3.525208	3.090567
5	2.193052	-3.104459	-0.161497
5	-2.560045	2.266309	2.424858
5	-0.275300	2.682164	-3.304735
5	-1.258939	0.187730	3.576243
5	-3.092416	-1.644401	-2.308119
5	-1.929433	-3.217341	1.531872
5	-0.434245	-4.004184	-0.624736
5	-4.042068	-1.320299	0.316689
5	4.042068	1.320299	-0.316689
5	-0.595519	-3.525208	-3.090567
5	3.092416	1.644401	2.308119
5	1.258939	-0.187730	-3.576243
5	0.976498	-1.279570	3.972453
5	0.939172	1.293508	4.038516
5	-0.976498	1.279570	-3.972453
5	1.929433	3.217341	-1.531872
5	-0.939172	-1.293508	-4.038516
6	-0.588800	0.020603	-1.375441
6	0.588800	-0.020603	1.375441
6	2.312152	0.870199	3.410974
6	-2.312152	-0.870199	-3.410974
5	-3.639069	1.007260	0.608231
5	-0.003618	2.933243	-1.400821
5	3.086165	1.113018	-1.936644
5	0.695758	-2.445617	-1.971739
5	-2.496008	-2.052913	-0.448526
5	0.003618	-2.933243	1.400821
5	3.639069	-1.007260	-0.608231
5	2.496008	2.052913	0.448526
5	-0.695758	2.445617	1.971739
5	-3.086165	-1.113018	1.936644
5	1.086587	0.038469	2.797581
5	-1.086587	-0.038469	-2.797581
7	-2.288156	0.778097	-3.328266

6	-0.145625	0.003529	-4.210174
6	0.145625	-0.003529	4.210174
7	2.288156	-0.778097	3.328266
6	-2.406404	2.977353	-1.518173
6	2.406404	-2.977353	1.518173
6	-3.651475	-0.889022	-1.085700
6	3.651475	0.889022	1.085700
6	1.171919	2.483983	-2.737071
6	-1.171919	-2.483983	2.737071
6	1.551505	-1.851878	-3.411740
6	-1.551505	1.851878	3.411740
6	-1.427937	-3.866636	-1.901778
6	1.427937	3.866636	1.901778
7	-3.152418	2.314038	1.155712
6	-3.238664	0.602896	-0.835495
6	3.238664	-0.602896	0.835495
7	3.152418	-2.314038	-1.155712
7	0.951882	3.910882	-0.710057
6	-1.245018	3.315318	-2.215972
6	1.245018	-3.315318	2.215972
7	-0.951882	-3.910882	0.710057
7	4.055827	0.231056	-1.333835
6	1.754188	0.987413	-2.672482
6	-1.754188	-0.987413	2.672482
7	-4.055827	-0.231056	1.333835
7	1.028220	-3.631654	-0.977411
6	0.206283	-2.487220	-3.658435
6	-0.206283	2.487220	3.658435
7	-1.028220	3.631654	0.977411
7	-3.178940	-2.385864	1.074664
6	-2.478982	-2.990852	-1.694385
6	2.478982	2.990852	1.694385
7	3.178940	2.385864	-1.074664