Supporting Materials

to accompany

A Monte Carlo Study of Isomers and Structural Evolution in Benzene-Cyclohexane Clusters: $(C_6H_6)(C_6H_{12})_n$, n = 3-7, 12.

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All supporting materials in this file are referenced in the primary manuscript. Brief narrative sections are included here to enhance organizational clarity. The contents of this supplement are arranged as follows:

S. A. Structures and Energies of Individual BC_n Isomers: BC_3 Major Isomers

Tables S1-S6 document the mean molecular coordinates for the five *major* **BC_3** isomers 1A, 1B, 2, 3, 4, and 5, respectively, resulting from the MC simulations. Also tabulated for each PES are the corresponding molecular coordinates, the optimized energies, and the mean-square displacement of the PES's atomic coordinates relative to the mean structure's coordinates. Isomer 1A is derived from the Jorgenson and Shi PESs, whereas Isomer 1B is based on the van de Waal and Williams PESs. Mean structures for BC_3 Isomers 2-5 are based on all four PESs. **Table S7** gives molecular stabilization energies by PES; the relative distribution of stabilization energies is provided for individual isomers in **Tables S8-S13.** The five major isomers of BC_3 are classified into three structural groups. Within each group, the average distance and angle deviations for each simulated structure vs. the model tetrahedron are tabulated in **Table S14**. Unless noted otherwise, distances are in angstroms, and angles are in radians. Similar documentation for the six *minor* BC_3 isomers is included in **Section S. G.** (page 40) of these supplemental materials.

Table S1. Molecular coordinates for Isomer 1A, based on the Jorgensen and Shi PESs only. The optimized energy and mean-square displacement of each PES's structural coordinates—relative to the mean structure—are shown for each PES.

Isomer 1A	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ	E (kJ mol^{-1})	$\langle(\Delta r)^2\rangle$
Jorgensen	1	4.296	0.251	-0.094	2.077	0.248	1.730	-56.15	0.014
	2	5.703	1.274	5.648	0.755	1.221	2.845		
	3	5.511	1.142	4.615	1.273	1.329	4.152		
Shi	1	4.317	0.240	0.069	2.074	0.361	1.746	-48.24	0.013
	2	5.707	1.241	5.651	0.780	1.258	2.837		
	3	5.490	1.101	4.603	1.292	1.295	4.128		
Mean	1	4.307	0.246	-0.013	2.075	0.305	1.738		
	2	5.705	1.258	5.650	0.768	1.240	2.841		
	3	5.501	1.122	4.609	1.283	1.312	4.140		
Standard Deviation	1	0.015	0.008	0.116	0.002	0.080	0.011		
	2	0.003	0.024	0.003	0.018	0.026	0.006		
	3	0.015	0.029	0.009	0.014	0.024	0.017		

Table S2. Molecular coordinates for Isomer 1B, based on the van de Waal and Williams PESs only. The optimized energy and mean-square displacement of each PES's structural coordinates—relative to the mean structure—are shown for each PES.

Isomer 1B	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ	E (kJ mol^{-1})	$\langle(\Delta r)^2\rangle$
van de Waal	1	4.488	0.174	0.487	2.083	0.495	1.777	-48.97	0.007
	2	5.888	1.155	5.674	0.839	1.361	2.811		
	3	5.709	1.041	4.561	1.363	1.288	4.109		
Williams	1	4.438	0.186	0.306	2.075	0.473	1.785	-49.68	0.007
	2	5.838	1.178	5.668	0.814	1.334	2.833		
	3	5.639	1.064	4.580	1.345	1.294	4.113		
Mean	1	4.463	0.180	0.396	2.079	0.484	1.781		
	2	5.863	1.167	5.671	0.826	1.347	2.822		
	3	5.674	1.052	4.571	1.354	1.291	4.111		
Standard Deviation	1	0.036	0.008	0.128	0.005	0.016	0.006		
	2	0.035	0.017	0.004	0.017	0.019	0.015		
	3	0.050	0.016	0.013	0.012	0.004	0.003		

Table S3. Molecular coordinates for Isomer 2, based on all four PESs. Also included for each PES is the optimized energy and mean-square displacement values. Results from an independent MP2 electronic structure optimization are shown in the bottom three rows.

Isomer 2	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ	E (kJ mol^{-1})	$\langle(\Delta r)^2\rangle$
Jorgensen	1	4.362	0.390	0.247	5.953	0.170	5.003	-50.18	0.010
	2	4.362	2.752	0.243	5.956	0.173	1.857		
	3	5.341	1.571	0.426	1.572	1.570	3.840		
Shi (3)	1	4.372	0.392	0.241	6.021	0.195	4.924	-44.04	0.011
	2	4.374	2.751	0.234	6.027	0.201	1.773		
	3	5.348	1.572	0.415	1.572	1.569	3.810		
van de Waal	1	4.507	0.373	0.306	6.045	0.125	4.905	-44.80	0.023
	2	4.509	2.767	0.303	6.033	0.125	1.776		
	3	5.634	1.570	0.433	1.571	1.571	3.834		
Williams	1	4.466	0.381	0.267	6.051	0.163	4.898	-45.44	0.004
	2	4.467	2.761	0.256	6.050	0.169	1.753		
	3	5.527	1.571	0.415	1.574	1.569	3.785		
Mean	1	4.427	0.384	0.262	6.016	0.165	4.933		
	2	4.427	2.758	0.262	6.016	0.165	1.792		
	3	5.462	1.571	0.422	1.571	1.571	3.817		
Standard Deviation	1	0.071	0.009	0.029	0.045	0.029	0.048		
	2	0.072	0.008	0.031	0.041	0.031	0.046		
	3	0.143	0.001	0.009	0.001	0.001	0.025		
MP2/6-31g(d)	1	4.183	0.315	0.364	2.936	0.133	4.949		2.9
	2	4.183	2.827	0.365	2.935	0.134	1.807		
	3	5.381	1.571	0.439	1.572	1.571	5.598		

Table S4. Molecular coordinates for Isomer 3, based on all four PESs, along with optimized energy and mean-square displacement values for each PES. Results from an independent MP2 electronic structure optimization are shown in the bottom three rows. *The next closest match is Isomer 5 with $\langle(\Delta r)^2\rangle = 1.9$.

Isomer 3	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ	E (kJ mol^{-1})	$\langle(\Delta r)^2\rangle$
Jorgensen	1	4.353	0.220	3.599	2.047	0.512	1.993	-56.04	0.014
	2	5.458	1.022	5.603	0.718	1.576	2.924		
	3	5.634	1.198	4.515	1.419	1.555	4.208		
Shi (3)	1	4.361	0.253	3.557	2.058	0.548	1.998	-48.44	0.023
	2	5.447	1.007	5.602	0.725	1.608	2.951		
	3	5.656	1.202	4.515	1.439	1.560	4.214		
van de Waal	1	4.516	0.209	3.508	2.071	0.556	1.993	-49.03	0.021
	2	5.696	1.018	5.627	0.749	1.594	2.944		
	3	5.906	1.181	4.524	1.436	1.537	4.222		
Williams	1	4.470	0.188	3.593	2.082	0.546	1.967	-49.61	0.015
	2	5.659	1.034	5.621	0.733	1.573	2.946		
	3	5.815	1.183	4.529	1.426	1.530	4.202		
Mean	1	4.424	0.217	3.563	2.065	0.541	1.987		
	2	5.564	1.020	5.614	0.731	1.588	2.941		
	3	5.753	1.191	4.521	1.430	1.546	4.212		
Standard Deviation	1	0.081	0.027	0.042	0.016	0.019	0.014		
	2	0.131	0.011	0.013	0.013	0.017	0.012		
	3	0.130	0.011	0.007	0.009	0.014	0.009		
MP2/6-31g(d)	1	4.296	0.252	3.602	3.158	0.476	1.147		1.2*
	2	5.506	1.042	5.602	0.714	1.546	3.356		
	3	5.704	1.240	4.517	1.733	1.604	5.192		

Table S5. Molecular coordinates for Isomer 4, based on all four PESs, along with optimized energy and mean-square displacement values for each PES.

Isomer 4	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**	**E (kJ mol^{-1})**	**$\langle(\Delta r)^2\rangle$**
Jorgensen	1	5.118	0.823	1.001	0.262	1.115	1.322	-55.07	0.019
	2	4.795	0.445	3.417	1.223	2.522	3.641		
	3	5.201	0.825	5.747	0.065	1.390	5.700		
Shi (3)	1	5.130	0.814	1.024	0.229	1.117	1.341	-47.89	0.009
	2	4.808	0.468	3.394	1.229	2.514	3.641		
	3	5.199	0.803	5.738	0.078	1.373	5.697		
van de Waal	1	5.377	0.826	1.019	0.219	1.127	1.314	-48.73	0.031
	2	4.974	0.481	3.321	1.238	2.545	3.612		
	3	5.398	0.790	5.726	0.073	1.346	5.655		
Williams	1	5.300	0.815	1.017	0.231	1.118	1.340	-49.20	0.008
	2	4.929	0.458	3.419	1.205	2.508	3.614		
	3	5.379	0.812	5.744	0.074	1.377	5.690		
Mean	1	5.231	0.820	1.015	0.235	1.120	1.329		
	2	4.875	0.463	3.386	1.224	2.522	3.627		
	3	5.294	0.807	5.739	0.072	1.372	5.686		
Standard Deviation	1	0.128	0.006	0.010	0.018	0.005	0.014		
	2	0.089	0.015	0.046	0.014	0.016	0.016		
	3	0.109	0.015	0.009	0.005	0.018	0.021		

Table S6. Molecular coordinates for Isomer 5, based on all four PESs, along with optimized energy and mean-square displacement values for each PES.

Isomer 5	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**	**E (kJ mol^{-1})**	**$\langle(\Delta r)^2\rangle$**
Jorgensen	1	5.952	2.036	5.697	4.752	1.709	0.720	-55.59	0.027
	2	5.662	1.930	4.779	3.592	1.443	4.277		
	3	4.392	2.935	3.979	2.126	0.565	5.301		
Shi (3)	1	5.934	2.067	5.718	4.807	1.693	0.760	-48.34	0.016
	2	5.658	1.950	4.788	3.564	1.455	4.281		
	3	4.390	2.921	3.814	2.162	0.603	5.304		
van de Waal	1	6.164	2.062	5.713	4.801	1.696	0.704	-48.51	0.023
	2	5.910	1.956	4.757	3.558	1.474	4.285		
	3	4.534	2.950	3.759	2.151	0.597	5.297		
Williams	1	6.114	2.055	5.723	4.796	1.688	0.730	-49.51	0.009
	2	5.824	1.961	4.783	3.567	1.477	4.281		
	3	4.503	2.956	3.829	2.152	0.598	5.297		
Mean	1	6.041	2.055	5.713	4.789	1.696	0.728		
	2	5.764	1.949	4.777	3.570	1.462	4.281		
	3	4.455	2.940	3.845	2.148	0.591	5.300		
Standard Deviation	1	0.116	0.013	0.012	0.025	0.009	0.023		
	2	0.125	0.014	0.014	0.015	0.016	0.003		
	3	0.075	0.016	0.094	0.015	0.018	0.004		

Table S7. Single-molecule energies for each major BC_3 isomer calculated on the relevant PESs. All entries are in kJ mol^{-1}.

Isomer	PES	Benzene	C_6H_{12} - 1	C_6H_{12} - 2	C_6H_{12} - 3
1A	Jorgensen	-13.29	-15.65	-13.81	-13.39
	Shi	-11.78	-13.43	-11.62	-11.41
1B	van de Waal	-12.05	-13.86	-11.58	-11.48
	Williams	-12.15	-14.05	-11.81	-11.68
2	Jorgensen	-15.77	-10.54	-10.54	-13.33
	Shi (3)	-14.05	-9.30	-9.29	-11.40
	van de Waal	-14.63	-9.62	-9.62	-10.92
	Williams	-14.62	-9.76	-9.76	-11.30
3	Jorgensen	-13.21	-15.51	-13.72	-13.60
	Shi (3)	-11.90	-13.47	-11.61	-11.47
	van de Waal	-12.12	-13.87	-11.66	-11.37
	Williams	-12.14	-14.04	-11.82	-11.62
4	Jorgensen	-13.48	-13.77	-14.29	-13.52
	Shi (3)	-12.24	-11.67	-12.50	-11.47
	van de Waal	-12.61	-11.76	-12.80	-11.56
	Williams	-12.60	-11.93	-12.95	-11.72
5	Jorgensen	-12.76	-13.54	-14.51	-14.78
	Shi (3)	-11.66	-11.48	-12.26	-12.94
	van de Waal	-11.88	-11.37	-11.94	-13.32
	Williams	-11.92	-11.65	-12.45	-13.49

Table S8. For BC_3 Isomer 1A the relative single-molecule energies are tabulated as a percent of the total cluster energy. Mean values and standard deviations are provided in the last two rows.

PES	Benzene	C_6H_{12} - 1	C_6H_{12} - 2	C_6H_{12} - 3
Jorgensen	23.7%	27.87%	24.6%	23.9%
Shi	24.4%	27.83%	24.1%	23.7%
Mean	24.1%	27.85%	24.4%	23.8%
Std. Dev.	0.5%	0.03%	0.4%	0.1%

Table S9. For BC_3 Isomer 1B the relative single-molecule energies are tabulated as a percent of the total cluster energy. Mean values and standard deviations are provided in the last two rows.

PES	Benzene	C_6H_{12} - 1	C_6H_{12} - 2	C_6H_{12} - 3
van de Waal	24.60%	28.31%	23.64%	23.45%
Williams	24.45%	28.27%	23.77%	23.51%
Mean	24.53%	28.29%	23.70%	23.48%
Standard Deviation	0.11%	0.02%	0.09%	0.04%

Table S10. For BC_3 Isomer 2 the relative single-molecule energies are tabulated as a percent of the total cluster energy. Mean values and standard deviations are provided in the last two rows.

PES	Benzene	C_6H_{12} - 1	C_6H_{12} - 2	C_6H_{12} - 3
Jorgensen	31.4%	21.0%	21.0%	26.6%
Shi (3)	31.9%	21.1%	21.1%	25.9%
van de Waal	32.7%	21.5%	21.5%	24.4%
Williams	32.2%	21.5%	21.5%	24.9%
Mean	32.0%	21.3%	21.3%	25.4%
Standard Deviation	0.5%	0.3%	0.3%	1.0%

Table S11. For BC_3 Isomer 3 the relative single-molecule energies are tabulated as a percent of the total cluster energy. Mean values and standard deviations are provided in the last two rows.

PES	Benzene	C_6H_{12} - 1	C_6H_{12} - 2	C_6H_{12} - 3
Jorgensen	23.6%	27.7%	24.5%	24.3%
Shi (3)	24.6%	27.8%	24.0%	23.7%
van de Waal	24.7%	28.3%	23.8%	23.2%
Williams	24.5%	28.3%	23.8%	23.4%
Mean	24.3%	28.0%	24.0%	23.7%
Standard Deviation	0.5%	0.3%	0.3%	0.5%

Table S12. For BC_3 Isomer 4 the relative single-molecule energies are tabulated as a percent of the total cluster energy. Mean values and standard deviations are provided in the last two rows.

PES	Benzene	C_6H_{12} - 1	C_6H_{12} - 2	C_6H_{12} - 3
Jorgensen	24.5%	25.0%	26.0%	24.6%
Shi (3)	25.6%	24.4%	26.1%	24.0%
van de Waal	25.9%	24.1%	26.3%	23.7%
Williams	25.6%	24.2%	26.3%	23.8%
Mean	25.4%	24.4%	26.2%	24.0%
Standard Deviation	0.6%	0.4%	0.2%	0.4%

Table S13. For BC_3 Isomer 5 the relative single-molecule energies are tabulated as a percent of the total cluster energy. Mean values and standard deviations are provided in the last two rows.

PES	Benzene	C_6H_{12} - 1	C_6H_{12} - 2	C_6H_{12} - 3
Jorgensen	23.0%	24.4%	26.1%	26.6%
Shi (3)	24.1%	23.8%	25.4%	26.8%
van de Waal	24.5%	23.4%	24.6%	27.5%
Williams	24.1%	23.5%	25.1%	27.3%
Mean	23.9%	23.8%	25.3%	27.0%
Standard Deviation	0.7%	0.4%	0.6%	0.4%

Table S14. Relative (percent) deviations of distances and angles for each BC_3 structure, relative to the model tetrahedron.

Group	Structure	Distance % Dev.	Angle % Dev.
1	1A	9	14
	1B	9	14
	3	9	13
	5	11	17
2	4	5	5
3	2	25	46

S. B. Structures and Energies of Individual BC_n Isomers: BC_4

MC simulations for the **BC_4** clusters identified 23 distinct isomers that were classified into two major structural groups, each consisting of two subgroups. **Tables S15 – S18** list all the BC_4 isomers with their molecular coordinates *by subgroup*. **Table S19** gives the benzene-molecule and total-cluster stabilization energy values and percent ratios for all BC_4 structures. Distance and angle deviations from the model trigonal bipyramid are listed in **Table S20.**

Table S15. Molecular coordinates for BC_4 subgroup 1A structures. Structures 1, 3, 5 and 6 resulted from the Jorgenson PES; structures 8, 9, 11, 12 and 13 are from the Shi PES; structures 15 and 17 derive from van de Waal; and structure 22 comes from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
1	1	4.476	0.292	1.731	5.150	2.619	0.833
	2	5.760	1.459	1.700	3.168	2.100	5.278
	3	5.628	1.214	0.734	1.756	1.639	3.133
	4	5.241	2.237	1.091	2.359	0.077	0.872

3	1	5.978	1.203	3.768	3.591	1.339	2.480
	2	4.994	2.239	4.090	3.896	2.631	3.974
	3	4.442	0.171	4.868	1.958	0.565	1.139
	4	5.462	1.346	4.709	3.567	1.210	5.186
5	1	4.988	0.761	3.057	5.423	2.942	3.337
	2	5.852	1.708	3.712	0.510	1.120	4.075
	3	5.619	1.798	2.753	1.965	1.701	2.175
	4	4.324	2.743	3.798	1.123	0.028	5.971
6	1	4.253	0.291	2.650	2.848	3.057	3.540
	2	4.756	2.441	2.026	0.942	0.323	5.172
	3	5.742	1.494	2.522	0.076	1.078	3.204
	4	5.592	1.449	1.561	0.763	1.917	4.219
8	1	5.606	1.662	1.519	1.948	1.305	5.121
	2	5.305	0.951	0.793	4.819	0.238	5.498
	3	5.637	2.003	0.571	5.937	1.788	6.166
	4	4.425	2.819	1.928	0.983	2.633	3.781
9	1	5.709	1.949	5.587	0.970	2.788	4.936
	2	5.481	1.086	5.943	0.215	0.335	4.805
	3	4.533	2.925	0.785	6.200	0.658	0.035
	4	5.369	1.763	0.423	1.594	1.255	3.887
11	1	5.470	1.445	5.802	0.950	1.931	2.645
	2	4.989	2.400	6.200	6.185	0.275	0.037
	3	6.138	1.505	0.468	3.100	1.439	1.514
	4	4.312	0.362	0.617	2.171	3.108	0.802
12	1	4.837	2.377	0.984	5.600	0.382	4.037
	2	5.730	1.394	0.612	2.119	0.961	6.214
	3	5.571	1.446	1.588	1.463	1.839	5.206
	4	4.548	0.311	1.355	6.216	0.602	4.401
13	1	4.362	0.430	5.797	1.978	3.068	1.710
	2	5.867	1.472	5.788	4.803	2.032	6.203
	3	5.621	1.395	4.835	2.032	1.650	1.147
	4	4.869	2.452	5.147	2.012	0.286	5.313
15	1	6.104	1.530	3.673	5.576	2.043	3.199
	2	4.634	0.485	3.812	1.158	0.130	4.358
	3	5.886	1.466	4.626	5.257	1.575	5.144
	4	4.953	2.540	4.298	3.135	2.774	1.077
17	1	4.549	0.517	3.014	2.242	0.191	2.930
	2	6.093	1.659	3.671	0.398	1.121	4.115
	3	4.572	2.707	3.567	3.966	3.043	2.646
	4	5.893	1.711	2.716	2.038	1.594	2.174
22	1	5.676	1.592	3.660	1.098	1.712	0.574
	2	5.941	1.650	2.630	3.460	1.816	5.390
	3	4.954	2.561	3.204	5.308	2.691	0.189
	4	4.397	0.408	2.995	4.380	2.975	5.667

Table S16. Molecular coordinates for structures belonging to BC_4 subgroup 1B. Structures 14 and 16 resulted from the van de Waal PES while structure 21 comes from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
14	1	4.485	0.389	1.621	6.237	3.077	5.438
	2	6.086	1.594	1.632	3.134	1.737	4.081
	3	5.946	1.387	2.526	2.315	1.504	6.276
	4	4.967	2.499	2.194	0.443	2.887	4.401
16	1	5.753	1.450	1.561	1.119	1.905	4.738
	2	5.177	2.423	1.186	2.202	0.286	1.058
	3	6.036	1.586	0.534	6.109	1.276	0.103
	4	4.470	0.384	0.454	2.947	0.041	1.571
21	1	4.797	2.602	5.287	0.827	2.804	1.678
	2	4.821	0.561	5.187	5.482	2.825	5.677
	3	5.985	1.506	5.675	3.074	1.758	0.059
	4	5.980	1.653	4.795	5.324	1.745	0.989

Table S17. Molecular coordinates for BC_4 subgroup 2A structures. Structures 2 and 4 derive from the Jorgenson PES; structure 10 comes from Shi; structure 18 resulted from van de Waal; structures 20 and 23 resulted from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
2	1	8.344	2.792	0.643	4.702	2.789	1.222
	2	4.670	2.755	4.019	3.225	2.227	3.609
	3	5.772	2.335	5.907	0.701	1.872	2.744
	4	5.232	2.297	1.207	5.763	2.888	5.224
4	1	4.793	2.577	2.048	3.125	2.699	5.171
	2	5.581	2.427	5.917	5.061	1.755	3.377
	3	8.165	3.121	0.136	1.412	2.936	2.547
	4	5.073	2.371	4.377	5.459	2.042	4.192
10	1	5.398	2.381	3.025	1.482	2.636	6.184
	2	5.340	2.259	4.546	4.341	1.433	1.864
	3	7.790	3.017	3.633	1.869	3.009	1.364
	4	4.895	2.597	0.420	5.130	2.582	3.526
18	1	4.396	0.329	1.028	0.388	0.044	0.735
	2	6.134	0.936	4.862	6.233	1.245	2.313
	3	8.519	0.267	4.435	3.286	0.089	2.149
	4	5.647	0.965	3.710	3.884	1.365	3.192
20	1	5.786	2.362	2.504	2.066	1.624	1.522
	2	8.421	3.135	2.320	1.648	0.126	3.640
	3	4.864	2.599	0.022	3.107	2.731	3.151
	4	5.777	2.441	3.868	4.343	1.361	4.284
23	1	6.005	2.306	0.539	1.269	1.666	4.374
	2	8.675	2.615	5.783	2.074	2.854	6.087
	3	5.406	2.012	5.564	1.596	0.890	2.664
	4	5.097	2.969	3.828	2.721	1.769	6.257

Table S18. Molecular coordinates for BC_4 subgroup 2B structures. Structure 7 resulted from the Shi PES while structure 19 was calculated on the van de Waal PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
7	1	5.403	2.318	5.699	5.224	1.693	6.233
	2	5.675	2.178	2.537	4.930	1.589	3.285
	3	5.361	2.581	1.323	3.944	1.476	6.166
	4	5.485	2.519	4.300	4.996	1.353	3.350
19	1	6.375	1.269	1.608	4.655	1.721	0.516
	2	4.787	0.098	1.698	2.684	0.843	5.958
	3	5.789	1.074	3.515	2.560	1.489	4.150
	4	6.198	1.141	2.453	4.738	1.729	0.563

Table S19. Benzene energy (Ben. E.) and cluster energy (Cluster E.) values and ratios, and the ratio of benzene to total cluster stabilization are shown for all BC_4 structures. The last column identifies the relevant PES.

Group	Structure	Ben. E. (kJ/mol)	Ben. E ratio (%)	Cluster E. (kJ/mol)	Cluster E. ratio (%)	E_B / E_{tot} Ratio (%)	PES
1A	1	-17.01	93.5	-80.75	97.9	21.1	Jorgensen
	3	-17.31	96.2	-80.90	98.1	21.4	Jorgensen
	5	-17.48	96.0	-81.60	98.9	21.4	Jorgensen
	6	-18.20	100.0	-81.23	98.4	22.4	Jorgensen
	8	-15.50	97.8	-70.00	99.3	22.1	Shi
	9	-15.77	99.5	-69.92	99.2	22.6	Shi
	11	-15.73	99.2	-69.05	97.9	22.8	Shi
	12	-15.85	100.0	-70.51	100.0	22.5	Shi
	13	-15.80	99.6	-70.28	99.7	22.5	Shi
	15	-16.05	96.5	-71.23	100.0	22.5	van de Waal
	17	-16.63	100.0	-70.88	99.5	23.5	van de Waal
	22	-16.76	100.0	-71.26	97.7	23.5	Williams
1B	14	-16.20	97.4	-71.06	99.8	22.8	van de Waal
	16	-16.24	97.6	-70.76	99.3	22.9	van de Waal
	21	-16.08	95.9	-72.97	100.0	22.0	Williams
2A	2	-12.43	68.3	-81.56	98.8	15.2	Jorgensen
	4	-12.99	71.4	-82.50	100.0	15.7	Jorgensen
	10	-12.35	77.9	-69.83	99.0	17.7	Shi
	18	-12.26	73.7	-70.79	99.4	17.3	van de Waal
	20	-11.53	68.8	-72.18	98.9	16.0	Williams
	23	-11.35	67.7	-72.17	98.9	15.7	Williams
2B	7	-13.74	86.6	-66.96	95.0	20.5	Shi
	19	-14.20	85.4	-68.98	96.8	20.6	van de Waal

The following definitions apply to this table, as well as to **Tables S29, 42, 46** and **55**.

Ben. E Ratio: Ben. E. *relative to* the lowest Ben. E. value for the *same* PES. For example the Ben. E Ratio for Structure 1 is given by -17.01 (Ben. E.) / -18.20 (lowest Ben. E. for all Jorgensen PES structures) x 100 = 93.5%.

Cluster E Ratio: Cluster E. *relative to* the lowest Cluster E. value for the *same* PES. For example the Cluster E Ratio for Structure 1 is given by -80.75 (Cluster E.) / -82.50 (lowest Cluster E. for all Jorgensen PES structures) x 100 = 97.9%.

E_B / E_{tot}: Ben. E. relative to the total cluster energy.

Table S20. Deviations (Std. Dev.) of each BC_4 structure from the model trigonal bipyramid for distance (in angstroms) and angle (in degrees). Also included are deviations from the specific configurations in which benzene occupies the axial or equatorial positions.

Group	Structure	Distance (Std. Dev)	Axial (Std. Dev)	Equatorial (Std. Dev)	Angle (Std. Dev)	Axial (Std. Dev)	Equatorial (Std. Dev)
1A	1	0.39	1.05	0.50	6.9	8.4	6.0
	3	0.45	0.88	0.57	7.6	7.4	7.1
	5	0.47	0.97	0.59	7.6	7.5	6.9
	6	0.55	0.95	0.61	7.9	7.4	8.4
	8	0.37	1.10	0.49	5.9	8.4	5.8
	9	0.38	1.06	0.44	5.7	8.2	5.9
	11	0.55	0.82	0.67	8.0	7.4	8.3
	12	0.40	0.98	0.49	6.9	7.8	6.4
	13	0.48	0.94	0.60	7.9	7.3	7.1
	15	0.50	0.98	0.62	8.0	7.1	7.1
	17	0.64	0.95	0.72	8.7	6.8	9.4
	22	0.57	0.95	0.61	7.7	7.3	8.1
1B	14	0.56	1.01	0.67	8.6	7.3	8.3
	16	0.54	0.99	0.60	7.3	7.7	7.4
	21	0.48	1.05	0.59	8.1	7.5	7.3
2A	2	0.40	0.40	1.40	6.3	6.2	12.0
	4	1.05	0.30	1.34	10.5	7.6	12.1
	10	0.49	0.33	1.13	8.0	8.3	12.4
	18	0.53	0.64	1.50	7.9	9.1	13.3
	20	0.48	0.42	1.33	8.1	8.1	12.2
	23	0.27	0.35	1.41	4.6	5.3	11.8
2B	7	0.47	1.19	0.12	6.6	9.1	5.6
	19	0.52	1.15	0.62	8.0	7.7	9.0

S. C. Structures and Energies of Individual BC_n Isomers: BC_5

For **BC_5** clusters, 26 unique isomers were identified through MC simulations. These were divided into three major structural groups; Groups 1 and 3 were further subdivided into three and four subgroups respectively. **Tables S21 – S28** list the molecular coordinates for each BC_5 isomer belonging to subgroups 1A – 1C, Group 2, and subgroups 3A – 3D, respectively. The benzene and cluster stabilization energy values for all BC_5 isomers and their percentage ratios are located in **Table S29**. The distance and angle deviations for each BC_5 isomer from the model octahedral configuration are listed in **Table S30**.

Table S21. Molecular coordinates for BC_5 subgroup 1A structures. Structure 5 was calculated from the Jorgenson PES; structure 17 came from van de Waal; and structures 23, 25 and 26 were a product of the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
5	1	5.592	2.111	1.553	3.546	1.081	3.823
	2	4.461	2.638	3.343	2.074	2.942	2.607
	3	4.490	0.399	3.015	3.253	2.670	4.869
	4	5.497	1.574	2.425	4.116	1.533	5.817
	5	5.355	1.480	3.595	5.746	1.448	3.864
17	1	4.449	0.426	5.425	3.794	0.100	5.697
	2	6.094	1.572	4.678	5.522	2.088	1.103
	3	5.804	1.567	5.724	0.074	1.412	2.427
	4	4.694	2.606	4.772	2.137	2.920	5.617
	5	5.649	2.140	0.359	2.776	1.069	4.339
23	1	5.984	1.737	2.567	5.057	2.210	3.135
	2	4.723	2.721	1.704	3.202	2.633	5.205
	3	5.778	0.866	2.524	5.610	0.499	6.025
	4	5.051	0.627	0.840	3.727	2.472	2.694
	5	5.651	1.568	1.596	0.278	1.472	4.361
25	1	5.934	1.703	2.551	2.335	1.492	3.013
	2	5.083	2.469	1.752	5.607	2.754	5.437
	3	5.052	0.605	0.604	5.673	2.299	2.822
	4	5.635	1.451	1.534	2.035	1.267	1.596
	5	5.395	0.679	2.737	5.659	0.626	6.056
26	1	5.610	1.649	0.495	3.978	1.581	0.703
	2	5.469	0.920	5.981	5.551	0.927	5.031
	3	5.937	1.723	1.571	0.123	0.908	5.229
	4	4.751	2.729	0.702	1.080	2.562	4.170
	5	4.910	0.711	1.484	2.916	0.364	0.815

Table S22. Molecular coordinates for BC_5 subgroup 1B. Structure 4 resulted from the Jorgenson PES; structure 11 from Shi, structure 19 from van de Waal, and structures 21 and 24 are from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
4	1	4.648	0.410	6.069	4.405	0.530	1.959
	2	6.034	1.922	4.751	3.486	0.105	2.625
	3	4.696	2.661	5.941	4.975	2.673	1.860
	4	5.918	1.142	4.696	1.975	0.058	2.075
	5	5.415	1.528	5.724	1.636	1.626	2.980
11	1	5.962	2.109	0.630	4.155	0.306	1.299
	2	4.368	0.018	0.633	3.064	2.570	1.148
	3	5.636	1.219	0.365	5.370	2.551	4.472
	4	5.365	1.740	5.813	0.443	1.817	5.449
	5	4.476	2.874	5.174	3.164	2.529	3.249
19	1	6.011	1.347	5.880	3.534	2.635	2.136
	2	4.466	0.406	0.985	1.219	0.119	1.750
	3	6.119	2.196	5.905	4.631	0.538	5.972
	4	4.890	2.645	1.247	2.504	0.600	5.950
	5	5.886	1.638	0.569	4.015	1.514	1.054
21	1	4.891	2.617	4.591	1.284	2.650	2.355
	2	4.670	0.380	4.261	3.368	2.612	5.564
	3	6.125	1.015	5.837	5.927	0.451	2.397
	4	5.961	1.843	5.791	0.465	0.438	3.015
	5	5.610	1.488	4.807	4.475	1.628	1.264
24	1	4.389	0.361	4.230	1.557	3.003	6.110
	2	5.092	2.514	3.759	6.198	1.129	0.123
	3	5.634	1.283	5.809	1.126	2.139	2.703
	4	5.843	1.532	4.778	4.233	1.333	4.251
	5	5.443	2.240	5.530	2.036	2.948	1.258

Table S23. Molecular coordinates for BC_5 subgroup 1C. The solo structure was calculated on the Jorgenson PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
2	1	4.943	0.618	3.074	0.545	2.598	1.666
	2	6.235	1.505	2.640	1.809	0.321	3.027
	3	5.207	2.330	2.817	0.647	0.384	1.524
	4	6.120	1.835	1.699	1.607	2.875	2.366
	5	5.797	1.053	1.591	1.200	2.996	1.947

Table S24. Molecular coordinates for BC_5 Group 2. Structure 3 resulted from the Jorgenson PES; structures 18 and 20 came from the van de Waal PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
3	1	7.903	2.702	0.411	1.031	2.993	1.275
	2	5.575	2.079	5.932	5.611	1.648	5.162
	3	4.203	2.906	3.137	6.233	0.072	4.427
	4	6.059	2.078	0.757	0.344	0.351	0.925
	5	5.659	1.271	0.292	2.801	2.692	4.110
18	1	8.749	2.572	5.748	0.074	2.877	5.525
	2	5.815	2.018	5.959	0.379	0.443	1.529
	3	4.407	0.372	6.179	4.909	0.065	5.553
	4	6.106	2.263	4.764	0.292	1.462	4.090
	5	5.139	3.011	1.469	5.820	1.460	2.187
20	1	6.547	1.706	3.645	3.435	0.969	4.622
	2	5.945	1.788	2.772	6.076	1.617	2.140
	3	4.663	0.593	3.036	4.893	2.816	6.088
	4	4.443	2.773	3.812	6.104	3.022	2.821
	5	9.124	2.289	3.345	3.111	0.610	0.238

Table S25. Molecular coordinates for BC_5 subgroup 3A; the solo structure was calculated on the Shi PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
14	1	5.536	1.432	3.670	5.067	1.522	3.213
	2	4.438	2.758	4.232	3.322	2.655	2.610
	3	5.794	1.624	4.610	4.873	2.230	5.175
	4	4.528	0.579	4.678	0.857	2.949	1.494
	5	5.485	1.976	5.657	0.128	1.884	6.255

Table S26. Molecular coordinates for BC_5 subgroup 3B. Structures 1 and 7 resulted from the Jorgenson PES; 8, 10 and 13 came from Shi; and structure 15 was calculated on the van de Waal PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
1	1	5.876	0.609	2.103	1.763	1.332	5.176
	2	5.550	0.685	3.793	2.264	1.194	1.904
	3	5.812	1.103	4.919	0.330	1.634	4.718
	4	8.586	0.066	4.521	5.788	0.326	0.450
	5	5.073	0.557	6.235	3.862	0.681	3.130
7	1	7.248	2.432	5.247	2.673	2.179	4.231
	2	8.461	2.494	0.259	0.212	2.548	0.066
	3	4.212	2.825	1.158	1.181	3.132	1.132
	4	6.282	1.846	0.502	5.701	2.230	4.376
	5	6.050	1.904	5.947	4.694	1.343	1.513
8	1	5.024	0.231	3.796	1.938	2.000	3.564
	2	5.737	0.832	0.239	1.734	2.534	0.570
	3	8.108	0.506	1.356	4.385	2.845	4.463
	4	6.257	1.574	0.601	4.451	0.452	3.688
	5	5.328	1.171	1.634	2.519	2.202	4.262
10	1	5.097	0.857	1.520	4.243	2.527	3.670
	2	5.573	0.787	6.001	2.357	1.525	3.111
	3	5.797	1.103	2.800	0.005	1.767	2.577
	4	7.718	0.108	1.228	2.936	0.172	3.391
	5	4.799	0.584	4.118	2.130	0.417	0.678
13	1	5.632	2.082	1.205	1.742	1.560	4.272
	2	7.878	2.769	2.948	2.126	0.368	5.210
	3	4.730	2.892	5.751	0.410	0.823	5.875
	4	5.508	2.090	2.470	5.772	0.524	0.559
	5	5.921	2.155	3.643	5.960	1.447	4.302
15	1	8.456	0.397	1.015	1.512	0.495	0.953
	2	6.109	1.444	1.671	4.163	2.184	1.495
	3	5.393	0.749	2.331	4.942	0.523	4.411
	4	4.974	0.479	5.116	2.102	0.945	4.881
	5	5.532	1.067	0.576	5.387	2.503	3.844

Table S27. Molecular coordinates for BC_5 subgroup 3C. Structure 6 came from the Jorgenson PES and 16 came from the van de Waal PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
6	1	8.220	0.253	3.437	0.202	0.149	6.113
	2	4.259	0.350	6.037	0.261	0.103	5.948
	3	5.804	1.191	4.866	4.159	1.866	4.440
	4	5.527	0.905	2.626	3.243	1.648	5.100
	5	5.914	1.007	3.798	3.364	1.530	5.682
16	1	5.979	0.905	4.994	5.896	0.505	1.532
	2	4.560	0.473	1.009	0.438	2.985	3.716
	3	8.390	0.228	4.662	6.179	2.843	2.869
	4	5.922	0.863	3.670	0.965	1.571	2.426
	5	8.439	0.597	2.653	4.062	1.953	5.442

Table S28. Molecular coordinates for BC_5 subgroup 3D structures. Structures 9 and 12 were both calculated on the Shi PES and 22 comes from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
9	1	5.377	0.847	0.898	4.076	0.310	3.731
	2	5.050	0.380	4.221	4.699	1.152	1.950
	3	8.125	0.306	1.474	3.275	0.157	1.405
	4	5.684	0.889	2.543	5.198	1.473	5.149
	5	5.613	1.024	5.878	1.239	1.535	2.192
12	1	8.350	0.726	4.956	3.438	1.308	4.874
	2	5.299	0.806	4.053	4.943	0.661	5.545
	3	5.118	0.734	1.955	1.451	2.719	2.410
	4	5.252	0.745	6.001	5.636	0.508	3.705
	5	7.533	0.018	3.339	2.744	2.975	4.396
22	1	5.414	0.775	4.841	5.433	1.862	1.127
	2	5.051	0.503	0.628	3.329	2.436	0.903
	3	8.664	0.764	3.803	6.257	1.641	0.744
	4	8.689	0.079	3.629	1.167	0.260	5.717
	5	5.825	0.760	2.934	5.312	1.888	1.190

Table S29. Benzene energy (Ben. E.) and cluster energy (Cluster E.) values and ratios, and the ratio of benzene to total cluster stabilization are shown for all BC_5 structures. The last column identifies the relevant PES.

Group	Structure	Ben. E. (kJ/mol)	Ben. E ratio (%)	Cluster E. (kJ/mol)	Cluster E. ratio (%)	E_B / E_{tot} Ratio (%)	PES
1A	5	-22.22	100.0	-104.18	97.0	21.3	Jorgensen
	17	-19.90	100.0	-92.01	99.5	21.6	van de Waal
	23	-19.42	95.4	-95.58	100.0	20.3	Williams
	25	-18.99	93.3	-94.17	98.5	20.2	Williams
	26	-19.64	96.5	-93.99	98.3	20.9	Williams
1B	4	-20.78	93.5	-107.19	99.8	19.4	Jorgensen
	11	-20.40	100.0	-88.77	97.5	23.0	Shi
	19	-19.77	99.3	-92.51	100.0	21.4	van de Waal
	21	-19.36	95.1	-94.76	99.1	20.4	Williams
	24	-20.36	100.0	-91.84	96.1	22.2	Williams
1C	2	-17.86	80.4	-104.46	97.3	17.1	Jorgensen
2	3	-17.01	76.6	-107.35	100.0	15.8	Jorgensen
	18	-17.00	85.4	-85.18	92.1	20.0	van de Waal
	20	-16.33	82.0	-90.56	97.9	18.0	van de Waal
3A	14	-19.52	95.7	-90.89	99.8	21.5	Shi
3B	1	-14.01	63.1	-106.90	99.9	13.1	Jorgensen
	7	-12.89	58.0	-107.07	99.7	12.0	Jorgensen
	8	-14.00	68.6	-88.56	97.2	15.8	Shi
	10	-14.86	72.7	-90.27	99.1	16.5	Shi
	13	-14.10	69.1	-90.30	99.2	15.6	Shi
	15	-15.27	76.7	-90.24	97.6	16.9	van de Waal
3C	6	-16.53	74.4	-104.82	97.6	15.8	Jorgensen
	16	-12.58	63.2	-91.27	98.7	13.8	van de Waal
3D	9	-14.85	72.8	-91.07	100.0	16.3	Shi
	12	-12.67	62.1	-90.13	99.0	14.1	Shi
	22	-12.22	60.0	-93.93	98.3	13.0	Williams

Table S30. Distance and angle deviations of each BC_5 structure, relative to the model octahedron. Distances are in angstroms and angles are in degrees.

Group	Structure	Distance (Std. Dev.)	Angle (Std. Dev.)
1A	5	0.78	17
	17	0.75	20
	23	0.76	28
	25	0.78	24
1B	4	0.73	32
	11	0.70	36
	19	0.73	29
	21	0.72	30
	24	0.74	23
1C	2	0.61	23
2	3	0.48	27
	18	0.60	32
	20	0.58	30
3A	14	0.73	8
3B	1	0.59	9
	7	0.76	18
	8	0.56	18
	10	0.53	7
	13	0.50	11
	15	0.53	13
3C	6	0.53	17
	16	0.89	21
3D	9	0.55	10
	12	0.78	24
	22	0.99	23

S. D. Structures and Energies of Individual BC_n Isomers: BC_6

All 28 structures resulting from the **BC_6** simulations were unique. These were classified into four major structural groups. Groups 1 and 4 were each further divided into three subgroups; Groups 2 and 3 were divided into two subgroups. Molecular coordinates for all BC_6 isomers are arranged by subgroup in **Tables S31 – S40**. BC_6 isomer structures were compared to the model pentagonal bipyramid. The center of mass to molecule (CM-to-molecule) distance, molecule-to-molecule distance, and angle (axial and equatorial) deviations for each isomer relative to the model structure are listed in **Table S41**. **Table S42** contains the benzene and cluster stabilization energy values for each BC_6 isomer.

Table S31. Molecular coordinates for BC_6 subgroup 1A. Structure 11 comes from the Shi PES and structure 27 is derived from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
11	1	5.740	2.196	1.625	6.212	0.486	0.762
	2	5.175	0.533	0.528	5.454	1.250	5.192
	3	5.636	1.205	1.470	0.772	1.332	2.213
	4	5.620	1.326	5.914	6.083	1.633	2.135
	5	4.564	2.628	6.028	3.561	2.584	4.847
	6	5.706	1.711	0.644	1.987	1.633	0.181
27	1	5.947	1.778	2.593	2.967	1.510	0.098
	2	4.592	2.639	1.600	5.943	0.067	4.983
	3	5.710	0.745	0.516	2.663	0.707	3.655
	4	5.584	1.478	1.617	5.170	1.869	4.666
	5	4.861	0.539	2.571	0.437	0.723	3.648
	6	5.686	1.698	0.486	4.351	1.237	3.520

Table S32. Molecular coordinates for BC_6 subgroup 1B. Both structures resulted from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
21	1	5.504	0.905	3.953	1.511	1.979	6.266
	2	5.864	2.006	4.600	4.740	2.325	3.732
	3	4.394	2.840	0.702	3.689	0.009	0.268
	4	6.712	1.241	4.991	4.446	0.105	2.853
	5	4.504	0.479	0.025	5.573	2.991	3.435
	6	6.057	1.740	5.698	4.432	0.610	3.387
28	1	6.099	1.216	0.556	4.850	1.454	4.454
	2	5.798	1.294	5.887	2.947	2.190	1.977
	3	5.448	1.862	1.457	1.302	1.216	4.907
	4	4.670	2.833	2.740	5.142	2.392	3.975
	5	4.585	0.193	0.643	4.133	0.660	3.384
	6	5.581	2.166	0.240	5.149	0.396	1.926
	5	4.861	0.539	2.571	0.437	0.723	3.648

Table S33. Molecular coordinates for BC_6 subgroup 1C. Structures 2 and 5 resulted from the Jorgenson PES, structure 14 from Shi; structure 17 from van de Waal; and structures 20, 25, and 26 from Williams.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
2	1	4.422	0.313	3.076	0.062	0.457	4.891
	2	5.370	1.456	2.718	0.484	1.393	2.490
	3	4.223	2.825	2.055	4.297	0.073	0.747
	4	6.445	1.801	1.695	2.904	0.047	5.639
	5	5.924	1.060	1.447	2.164	2.893	1.443
	6	5.404	1.732	0.663	0.750	1.900	0.277
5	1	5.790	1.643	2.753	4.146	1.092	5.184
	2	6.252	1.824	3.680	1.617	0.894	4.263
	3	4.240	0.305	6.283	5.388	0.089	0.740
	4	5.861	0.949	3.402	1.440	0.407	0.359
	5	5.617	1.135	4.547	0.252	1.663	5.122
	6	4.212	2.818	3.521	3.740	3.103	3.934
14	1	5.921	1.327	4.571	3.741	1.930	4.302
	2	5.387	1.955	3.680	4.133	1.897	3.239
	3	5.632	2.249	5.028	5.321	2.556	1.068
	4	4.286	0.325	4.226	4.223	0.180	2.201
	5	5.562	1.231	5.554	0.787	1.382	6.203
	6	4.449	2.889	2.213	5.223	2.461	1.204
17	1	4.645	0.179	4.235	3.056	2.476	5.216
	2	5.623	1.332	4.790	2.532	1.916	1.244
	3	6.555	1.931	5.632	3.621	0.414	0.653
	4	4.545	2.933	5.147	3.134	2.556	3.425
	5	5.558	1.910	0.471	5.926	2.052	0.958
	6	5.925	1.157	5.954	4.117	0.188	0.346
20	1	5.504	0.905	3.953	1.511	1.979	6.266
	2	5.864	2.006	4.600	4.740	2.325	3.732
	3	4.394	2.840	0.702	3.689	0.009	0.268
	4	6.712	1.241	4.991	4.446	0.105	2.853
	5	4.504	0.479	0.025	5.573	2.991	3.435
	6	6.057	1.740	5.698	4.432	0.610	3.387
25	1	5.476	1.880	2.544	5.579	1.144	6.060
	2	4.631	2.942	3.767	4.134	0.745	2.075
	3	5.964	1.268	1.782	4.101	0.472	1.021
	4	4.478	0.164	2.597	4.156	0.612	4.085
	5	5.736	2.095	1.340	4.367	2.827	6.253
	6	5.614	1.077	0.653	3.535	1.324	0.030
26	1	4.561	0.251	4.033	1.206	2.656	4.400
	2	4.960	2.580	4.200	3.995	0.708	5.767
	3	5.499	1.923	5.578	5.952	0.992	2.882
	4	5.836	1.310	3.894	1.609	1.345	0.172
	5	7.691	1.788	4.689	4.329	0.935	1.207
	6	6.352	1.142	4.963	5.808	0.447	1.613

Table S34. BC_6 subgroup 2A molecular coordinates, calculated on the Jorgenson PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
4	1	4.621	0.618	6.140	2.166	2.858	3.036
	2	6.006	2.090	4.535	0.068	0.501	5.330
	3	4.386	2.855	6.192	3.075	2.722	1.827
	4	5.762	1.283	4.668	5.569	0.338	4.445
	5	5.495	1.734	5.622	3.282	1.377	2.792
	6	5.710	1.599	0.415	4.295	1.192	4.136

Table S35. Molecular coordinates of BC_6 subgroup 2B. Structure 6 came from the Jorgenson PES, structures 18 and 19 from van de Waal; and structures 22 and 23 came from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
6	1	7.801	0.156	5.362	1.790	0.468	4.779
	2	5.810	0.914	5.078	3.121	0.714	2.681
	3	5.789	1.735	4.510	2.375	0.971	0.837
	4	4.407	0.558	1.002	0.218	0.216	0.927
	5	4.995	0.868	3.619	3.510	0.787	3.645
	6	5.806	1.647	5.497	0.090	0.932	3.088
18	1	8.935	2.475	5.689	3.301	2.683	0.947
	2	6.307	1.893	5.834	1.897	0.024	3.140
	3	5.303	0.942	5.813	5.332	2.596	2.686
	4	5.817	2.310	4.600	5.884	1.591	1.691
	5	4.419	2.790	0.977	2.953	0.066	5.230
	6	5.824	1.541	0.522	3.642	1.543	0.984
19	1	6.184	1.059	0.442	1.375	1.920	2.177
	2	4.371	0.253	3.128	1.959	3.100	0.771
	3	6.458	1.926	0.774	2.427	0.234	1.786
	4	4.648	2.936	0.914	1.039	2.493	3.444
	5	6.145	1.139	1.390	5.120	1.472	5.249
	6	10.050	1.408	0.832	1.375	1.680	4.186
22	1	5.483	1.774	1.456	5.754	1.274	4.927
	2	5.060	0.560	1.215	5.097	2.456	5.940
	3	6.360	1.354	0.476	0.284	2.989	2.702
	4	4.402	2.947	3.433	0.972	2.758	1.889
	5	6.154	2.149	0.332	5.458	2.647	3.034
	6	8.055	2.579	1.126	1.157	2.700	1.944
23	1	4.327	2.827	1.921	0.191	3.109	3.185
	2	4.726	0.364	3.812	1.086	2.550	3.901
	3	5.829	0.969	1.379	2.293	1.489	2.278
	4	5.667	1.847	0.668	1.993	1.797	0.224
	5	5.927	0.851	0.150	6.008	0.789	2.912
	6	8.184	0.210	0.786	1.918	3.015	3.730

Table S36. Molecular coordinates of BC_6 subgroup 3A, calculated on the van de Waal PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
15	1	10.206	1.497	2.046	2.228	1.148	4.969
	2	5.685	2.099	1.885	1.182	0.116	4.787
	3	6.475	1.428	2.617	5.053	0.525	1.938
	4	4.404	0.270	3.082	0.821	3.079	1.380
	5	6.052	1.274	1.494	5.457	0.324	1.478
	6	8.536	0.882	2.152	0.484	2.568	5.727

Table S37. Molecular coordinates for BC_6 subgroup 3B structures. Structures 7 and 8 resulted from calculations on the Shi PES and structure 16 was calculated on the van de Waal PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
7	1	7.314	2.534	5.224	0.649	0.860	1.133
	2	8.225	2.540	0.348	4.470	2.285	6.241
	3	4.495	2.884	1.332	2.159	0.637	2.630
	4	5.840	1.751	0.430	2.507	1.221	1.169
	5	5.837	1.918	5.860	4.786	2.088	4.760
	6	5.280	0.926	5.988	2.070	0.263	5.083
8	1	8.446	0.148	4.256	3.535	0.555	3.754
	2	6.127	0.793	5.482	0.854	1.596	5.004
	3	8.663	0.564	0.494	0.407	2.850	1.682
	4	6.142	1.116	0.328	0.518	0.410	3.655
	5	4.295	0.276	1.934	1.457	2.939	1.033
	6	5.835	1.734	5.936	3.660	0.589	2.157
16	1	5.926	1.151	4.920	3.266	1.415	1.410
	2	5.562	0.788	6.139	5.944	0.440	2.931
	3	8.148	0.145	0.452	2.019	2.986	1.431
	4	4.796	0.589	3.443	1.025	2.944	0.449
	5	5.582	0.891	1.363	2.298	1.415	1.790
	6	6.136	1.650	5.883	0.595	2.348	6.129

Table S38. Molecular coordinates of BC_6 subgroup 4A, derived from the Shi PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
13	1	6.846	2.261	0.580	0.502	1.721	0.020
	2	8.138	2.926	1.368	4.311	0.407	5.664
	3	4.799	2.698	5.124	1.484	2.394	2.656
	4	5.241	2.228	1.663	2.927	0.572	3.457
	5	5.968	2.405	3.166	4.310	1.498	3.231
	6	5.761	1.914	5.809	3.240	1.146	5.735

Table S39. Molecular coordinates of BC_6 subgroup 4B, derived from the Shi PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
12	1	8.149	0.503	6.062	0.216	2.556	3.167
	2	5.344	0.923	5.082	0.784	0.393	3.758
	3	5.580	1.142	3.846	3.665	1.590	3.210
	4	5.087	0.232	2.028	1.439	1.338	2.679
	5	8.727	0.494	4.493	3.019	2.105	0.937
	6	5.541	1.069	0.291	4.338	0.065	5.531

Table S40. Molecular coordinates for BC_6 subgroup 4C structures. Structures 1 and 3 resulted from calculations on the Jorgenson PES, structures 9 and 10 from Shi, and structure 24 from the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
1	1	5.961	1.051	1.492	5.712	1.655	1.903
	2	5.226	0.583	2.979	5.518	2.441	2.917
	3	5.908	0.618	4.979	3.879	1.318	1.862
	4	8.632	0.036	1.526	5.737	0.332	3.467
	5	5.446	0.638	0.471	0.874	1.932	1.742
	6	5.846	1.396	5.949	1.597	1.135	2.212
3	1	7.751	2.802	4.692	1.427	3.018	2.074
	2	5.798	2.278	5.880	4.302	1.915	4.000
	3	5.615	2.154	4.553	2.124	2.805	0.316
	4	4.381	2.656	2.226	1.573	2.953	2.604
	5	6.104	1.962	0.708	4.712	3.010	3.552
	6	8.238	2.602	0.757	3.947	0.530	4.251
9	1	8.842	0.438	1.313	4.477	2.341	4.583
	2	5.167	0.823	4.339	3.870	0.239	1.886
	3	8.233	0.281	3.939	2.864	2.874	1.327
	4	5.657	0.737	2.635	6.265	1.523	5.707
	5	4.980	0.494	0.409	1.177	2.190	4.904
	6	5.772	1.133	5.546	3.007	1.393	2.841
10	1	8.756	0.345	0.974	6.029	1.520	4.158
	2	5.370	0.608	5.401	0.891	2.072	0.865
	3	5.462	0.597	2.351	5.997	2.113	3.270
	4	8.741	0.301	3.919	3.187	0.256	4.824
	5	5.879	0.915	3.925	4.557	1.100	0.805
	6	5.445	0.934	0.624	5.822	2.899	1.182
24	1	5.327	0.641	4.067	4.197	1.023	2.673
	2	5.426	0.797	5.961	3.952	0.298	2.914
	3	9.073	0.495	3.256	1.164	0.844	2.902
	4	5.564	0.564	1.710	0.232	1.648	4.786
	5	5.924	1.234	2.897	0.968	1.520	5.963
	6	8.633	0.216	5.954	0.082	0.303	5.742

Table S41. BC_6 structural deviations, compared to the model pentagonal bipyramid. Distances are in angstroms and angles are in degrees.

		Distance		Angle	
Group	Structure	CM-to-molecule (Std. Dev.)	Molecule-to-molecule (Std. Dev.)	Axial (Std. Dev.)	Equatorial (Std. Dev.)
1A	11	0.26	0.4	11	19
	27	0.36	0.5	8	21
1B	21	0.68	0.8	25	13
	28	0.60	0.6	27	12
1C	2	0.52	0.8	25	7
	5	0.46	0.8	32	11
	14	0.57	0.6	26	11
	17	0.52	0.7	27	8
	20	0.74	1.5	18	16
	25	0.59	0.6	26	11
	26	0.51	1.0	23	10
2A	4	0.37	0.6	11	20
2B	6	0.49	1.0	21	10
	18	0.62	1.4	29	4
	19	0.97	1.9	29	22
	22	0.70	1.2	32	16
	23	0.86	1.2	33	15
3A	15	0.45	1.9	27	11
3B	7	0.73	1.2	26	13
	8	0.71	1.5	23	15
	16	0.52	1.0	24	7
4A	13	0.61	1.1	15	15
4B	12	0.29	1.5	26	4
4C	1	0.73	1.1	19	11
	3	0.37	1.3	26	9
	9	0.62	1.5	21	8
	10	0.21	1.5	26	4
	24	0.24	1.6	24	5

Table S42. Benzene energy (Ben. E.) and cluster energy (Cluster E.) values and ratios, and the ratio of benzene to total cluster stabilization are shown for all BC_6 structures. The last column identifies the relevant PES.

Group	Structure	Ben. E (kJ/mol)	Ben. E Ratio (%)	Cluster E. (kJ/mol)	Cluster E. Ratio (%)	E_B / E_{tot} Ratio (%)	PES
1A	11	-21.00	90.5	-117.01	100.0	17.9	Shi
	27	-22.85	92.2	-119.36	100.0	19.1	Williams
1B	21	-23.46	98.2	-112.24	96.1	20.9	Williams
	28	-24.12	97.4	-118.40	99.2	20.4	Williams
1C	2	-25.31	100.0	-132.49	98.0	19.1	Jorgensen
	5	-25.28	99.9	-132.59	98.1	19.1	Jorgensen
	14	-23.19	100.0	-114.50	97.9	20.3	Shi
	17	-23.84	100.0	-116.83	100.0	20.4	van de Waal
	20	-19.08	80.0	-115.59	98.9	16.5	Williams
	25	-24.77	100.0	-118.68	99.4	20.9	Williams
	26	-19.54	78.9	-117.06	98.1	16.7	Williams
2A	4	-24.70	97.6	-135.21	100.0	18.3	Jorgensen
2B	6	-20.61	81.4	-130.39	96.4	15.8	Jorgensen
	18	-18.86	79.1	-110.86	94.9	17.0	van de Waal
	19	-19.36	81.2	-109.89	94.1	17.6	van de Waal
	22	-19.12	77.2	-114.62	96.0	16.7	Williams
	23	-21.06	85.0	-112.13	93.9	18.8	Williams
3A	15	-15.17	63.6	-115.08	98.5	13.2	van de Waal
3B	7	-17.42	68.8	-132.09	97.7	13.2	Shi
	8	-13.29	57.3	-109.15	93.3	12.2	Shi
	16	-18.50	77.6	-114.43	97.4	16.2	van de Waal
4A	13	-15.11	65.2	-114.12	97.5	13.2	Shi
4B	12	-15.03	64.8	-115.02	98.3	13.1	Shi
4C	1	-17.02	67.2	-130.87	96.8	13.0	Jorgensen
	3	-16.62	65.7	-133.69	98.9	12.4	Jorgensen
	9	-14.38	62.0	-114.88	98.2	12.5	Shi
	10	-13.79	59.5	-115.34	98.6	12.0	Shi
	24	-14.51	58.6	-118.45	99.2	12.2	Williams

S.E. Structures and Energies of Individual BC_n Isomers: BC_7

All 14 **BC_7** simulations were run on the Jorgenson PES; all resulting structures are unique. The isomers were classified into two groups. Group 1 was further divided into two subgroups. **Tables S43 – S45** provide the molecular coordinates for each BC_7 isomer by subgroup. **Table S46** contains the benzene and cluster stabilization energies for each BC_7 isomer. BC_7 clusters were evaluated against the model hexagonal bipyramid: the center of mass to molecule (CM-to-molecule) distance, molecule-to-

molecule distance, and angle (axial and equatorial) deviations, relative to the model structure, are listed in **Table S47**.

Table S43. Molecular coordinates for BC_7 subgroup 1A structures, all of which derive from the Jorgenson PES**.**

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
2	1	5.410	1.913	0.365	5.544	2.150	0.900
	2	5.589	1.118	6.049	1.228	0.246	5.851
	3	4.474	2.980	3.862	0.981	2.469	2.006
	4	5.377	0.959	4.553	5.073	0.270	3.153
	5	5.641	1.854	4.525	5.173	2.601	5.375
	6	8.144	1.427	5.278	1.523	1.947	0.799
	7	6.006	2.041	5.601	3.659	2.136	0.960
4	1	5.792	1.167	1.330	2.013	3.028	4.832
	2	8.337	1.710	1.916	4.520	1.775	5.377
	3	5.860	1.986	1.239	2.037	0.120	5.225
	4	6.059	2.117	2.554	5.456	2.634	5.301
	5	4.496	0.172	2.835	2.074	0.641	5.059
	6	5.907	1.297	2.552	2.871	2.736	0.375
	7	4.522	3.098	1.397	3.314	2.461	5.213
5	1	6.040	1.120	2.419	3.212	0.114	5.302
	2	4.173	3.099	1.300	2.127	3.109	1.020
	3	5.378	1.808	0.575	5.068	1.318	3.341
	4	6.508	1.453	1.468	6.122	0.359	3.317
	5	7.386	2.197	1.592	3.530	2.302	0.973
	6	4.340	0.472	0.758	2.369	2.923	3.385
	7	6.085	1.890	2.413	2.380	0.048	6.111
6	1	4.855	0.646	0.971	4.742	0.611	2.316
	2	5.682	1.845	1.431	4.524	1.627	2.135
	3	6.631	1.753	5.808	2.613	1.049	4.149
	4	5.697	1.567	0.537	5.223	1.797	6.215
	5	5.293	0.959	5.449	1.520	3.141	6.061
	6	5.570	1.814	4.894	1.039	2.121	4.333
	7	4.187	2.825	0.240	1.450	0.072	3.884
7	1	5.244	0.928	2.324	1.138	0.105	4.356
	2	5.786	1.671	3.630	2.289	1.305	6.092
	3	5.566	1.937	4.537	4.807	1.502	2.080
	4	4.811	0.786	4.254	0.506	2.731	1.212
	5	4.171	2.874	3.004	6.072	3.087	1.954
	6	5.596	1.739	1.707	1.061	2.015	1.155
	7	6.649	1.736	2.610	4.666	2.214	4.051

8	1	5.597	1.960	1.762	1.736	0.297	4.093
	2	4.403	2.877	0.057	1.098	2.607	4.665
	3	5.338	1.157	2.306	5.680	2.245	5.614
	4	4.995	0.003	1.855	4.695	1.727	5.894
	5	5.833	0.963	6.242	6.283	1.297	5.527
	6	6.035	1.770	0.538	1.362	0.499	3.099
	7	5.955	1.159	1.072	5.278	0.370	2.586
9	1	4.871	0.584	2.074	4.812	2.163	5.760
	2	5.934	0.985	0.604	2.432	2.697	0.557
	3	5.580	1.716	1.456	5.216	1.555	4.568
	4	5.391	0.440	5.085	5.877	1.725	5.215
	5	6.041	1.240	5.767	3.465	1.859	5.730
	6	4.195	2.826	0.855	1.250	3.126	1.191
	7	6.380	1.727	0.364	0.747	3.004	0.602
10	1	4.505	2.643	3.782	1.052	3.101	3.912
	2	5.988	1.665	3.647	4.642	0.995	3.956
	3	6.021	1.697	2.763	2.239	1.239	4.673
	4	8.570	1.331	4.180	3.965	0.776	4.350
	5	8.639	1.953	4.302	3.252	2.456	4.694
	6	4.925	0.633	3.825	1.983	0.442	0.894
	7	5.489	1.560	4.832	0.768	1.617	1.209
11	1	6.263	1.239	1.357	0.525	2.946	2.477
	2	5.288	1.264	2.473	5.659	2.062	5.984
	3	6.515	2.004	0.711	2.552	2.091	2.975
	4	6.101	1.954	1.751	3.359	0.195	1.833
	5	4.308	0.205	0.370	2.535	2.953	0.572
	6	6.232	1.352	0.277	5.205	2.510	2.331
	7	4.514	2.920	1.105	4.131	0.630	1.286
12	1	5.836	1.007	4.602	2.204	1.211	1.015
	2	9.191	1.528	4.484	4.414	1.973	1.042
	3	6.217	1.893	4.938	0.718	3.086	1.927
	4	6.215	1.229	5.562	0.518	1.438	0.532
	5	4.420	2.938	4.731	3.062	2.573	0.962
	6	4.613	0.133	5.694	4.649	0.809	1.528
	7	5.683	1.931	3.929	5.795	1.567	3.175
14	1	4.414	2.643	2.025	5.867	2.943	2.298
	2	7.698	1.379	3.661	5.461	0.647	4.352
	3	5.360	1.249	4.625	1.993	1.925	1.805
	4	4.376	0.433	3.156	1.103	0.178	3.310
	5	5.104	2.366	5.230	4.605	1.082	2.640
	6	5.594	1.566	2.839	0.089	1.500	5.626
	7	5.454	2.129	3.873	4.413	1.531	0.719

Table S44. Molecular coordinates for the solo subgroup 1B structure, which derives from the Jorgenson PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
3	1	4.782	0.474	1.763	3.208	2.525	1.773
	2	5.740	0.777	4.204	6.212	1.520	0.165
	3	5.597	1.735	4.805	5.365	1.496	1.805
	4	6.234	1.736	5.755	4.472	1.910	0.642
	5	5.561	1.709	3.760	2.882	1.847	3.193
	6	5.633	0.749	5.444	5.358	1.620	3.269
	7	4.231	2.874	4.942	2.970	3.037	2.901

Table S45. Molecular coordinates for BC_7 Group 2 structures, both of which derive from the Jorgenson PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
1	1	6.113	1.252	1.493	1.564	1.488	2.878
	2	9.050	0.041	5.283	2.400	0.993	2.592
	3	7.172	0.664	2.285	3.052	1.171	2.654
	4	9.403	0.602	0.123	3.518	1.292	5.848
	5	6.401	1.256	0.631	5.012	2.225	0.049
	6	8.856	0.694	1.113	1.589	2.533	3.115
	7	4.232	0.285	0.055	2.515	3.039	4.715
13	1	8.536	0.436	1.616	2.929	2.823	3.768
	2	6.171	1.080	1.385	2.237	0.927	5.177
	3	5.748	1.104	5.893	5.971	1.695	5.113
	4	7.575	0.936	0.514	4.848	2.280	1.680
	5	9.503	0.514	0.065	5.785	2.489	1.971
	6	4.539	0.008	6.003	0.472	0.718	1.599
	7	6.341	1.662	0.537	3.515	0.358	2.892

Table S46. Benzene energy (Ben. E.) and cluster energy (Cluster E.) values, and the ratio of benzene to total cluster stabilization are shown for all BC_7 structures. All of these structures were calculated on the Jorgensen PES.

Group	Structure	Benzene E. (kJ/mol)	Cluster E. (kJ/mol)	E_B / E_{tot} Ratio (%)
1A	2	-24.51	-162.73	15.1
	4	-24.23	-157.43	15.4
	5	-24.70	-159.39	15.5
	6	-27.61	-161.68	17.1
	7	-27.81	-160.93	17.3
	8	-26.96	-161.33	16.7
	9	-25.67	-158.33	16.2
	10	-20.64	-160.12	12.9
	11	-25.83	-159.30	16.2
	12	-22.64	-159.45	14.2
	14	-27.27	-160.04	17.0
1B	3	-27.71	-159.22	17.4
2	1	-12.69	-161.80	7.8
	13	-14.72	-162.12	9.1

Table S47. Structural deviations from the model hexagonal bipyramid for BC_7 structures. Distances are in angstroms and angles are in degrees.

		Distance		Angle	
Group	Structure	CM-to-molecule (Std. Dev.)	Molecule-to-molecule (Std. Dev.)	Axial (Std. Dev.)	Equatorial (Std. Dev.)
1A	2	0.40	1.1	25	16
	4	0.71	1.2	21	10
	5	0.42	1.1	29	16
	6	0.70	0.7	23	20
	7	0.66	0.7	24	19
	8	0.37	0.6	19	12
	9	0.33	0.7	22	13
	10	0.71	1.5	30	18
	11	0.46	0.8	26	16
	12	0.68	1.5	26	9
	14	0.36	1.0	26	15
1B	3	0.60	0.6	29	17
2	1	0.47	1.8	26	13
	13	0.44	1.6	29	18

S. F. Structures and Energies of Individual BC_n Isomers: BC_{12}

Monte Carlo simulations for BC_{12} clusters identified 20 distinct isomers, which were classified into six structural groups based on conformity to the model closed-shell icosahedron. **Tables S48 – S53** tabulate the molecular coordinates for BC_{12} isomers by group number. The CM-to-molecule distance, molecule-to-molecule distance, and angle deviations, relative to benzene occupying the interior vs. first shell positions of an icosahedron, are shown in **Table S54**. **Table S55** gives the benzene- and cluster-stabilization energies for all BC_{12} isomers.

Table S48. Molecular coordinates for BC_{12} Group 1 structures. Structure 1 was calculated on the Jorgenson PES, structure 6 on Shi, structures 11 and 14 on van de Waal, and 19 and 20 on the Williams PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
1	1	6.037	1.166	2.431	0.487	1.451	3.985
	2	5.417	1.815	1.600	3.886	1.062	4.825
	3	6.022	1.117	6.187	3.698	0.497	4.213
	4	5.488	2.181	2.861	1.234	0.916	6.054
	5	6.114	1.694	0.457	0.036	2.373	1.061
	6	5.431	1.173	4.929	0.761	0.923	4.711
	7	4.878	0.005	5.202	3.687	1.182	4.472
	8	5.256	1.207	3.589	2.044	1.941	0.468
	9	5.340	2.112	4.278	3.971	2.378	4.457
	10	5.444	2.092	5.603	2.059	1.366	2.639
	11	4.997	2.870	0.639	0.351	1.775	2.088
	12	5.877	0.928	1.228	4.354	0.666	5.025

6	1	5.602	2.507	4.558	1.792	2.193	1.777
	2	4.660	0.515	0.901	4.823	2.542	5.176
	3	6.475	1.643	4.624	1.286	1.363	4.079
	4	5.108	2.433	2.331	0.457	0.898	0.299
	5	5.635	1.687	1.420	1.394	1.562	4.749
	6	5.818	1.703	3.513	4.231	2.099	3.692
	7	5.210	1.195	2.523	1.699	2.046	5.923
	8	5.467	2.448	0.461	3.790	0.788	6.141
	9	5.577	0.781	4.026	0.025	1.736	5.995
	10	5.451	1.022	5.398	5.779	0.185	0.642
	11	6.173	1.848	5.523	3.545	3.137	4.531
	12	5.792	1.580	0.276	0.107	2.281	3.637
11	1	5.763	1.019	2.245	4.049	2.421	0.344
	2	5.582	0.757	0.580	3.184	1.833	4.875
	3	6.276	1.960	2.540	5.886	3.054	0.918
	4	5.931	2.309	5.513	2.039	1.207	1.034
	5	5.794	1.874	0.297	0.946	1.037	3.668
	6	5.199	0.421	4.320	5.776	2.222	3.881
	7	5.346	2.751	1.412	5.691	1.490	2.678
	8	5.757	1.230	5.698	5.917	1.914	2.664
	9	6.037	1.671	1.402	4.449	2.051	4.924
	10	5.760	1.367	3.406	6.154	1.273	3.601
	11	5.745	1.546	4.556	3.746	1.651	1.600
	12	5.986	2.329	3.857	0.600	2.389	1.196
14	1	5.367	2.704	2.557	1.564	2.060	5.791
	2	5.887	1.657	5.789	2.123	1.293	2.667
	3	5.425	0.793	1.779	4.336	0.283	4.527
	4	5.987	2.418	4.791	3.826	1.144	4.616
	5	5.757	1.413	4.721	2.115	1.145	4.650
	6	5.786	0.817	3.583	4.492	0.631	1.109
	7	5.786	1.683	2.587	1.273	1.528	5.817
	8	6.067	1.789	1.426	4.294	1.750	2.094
	9	5.730	2.396	0.359	5.429	2.287	2.631
	10	5.882	1.307	0.608	6.043	1.722	3.139
	11	5.981	1.808	3.761	4.036	1.665	3.124
	12	5.414	0.524	5.581	3.856	1.147	0.910
19	1	5.227	0.987	1.565	1.656	0.673	1.851
	2	5.439	0.786	3.345	5.190	2.707	3.774
	3	5.882	2.138	4.866	2.413	2.058	3.352
	4	5.759	2.143	1.369	4.085	1.546	5.015
	5	5.253	2.812	3.004	1.652	1.379	1.789
	6	5.688	1.714	3.824	4.161	1.312	0.488
	7	6.080	1.485	0.390	0.358	1.277	0.884
	8	6.160	1.470	5.647	4.370	2.185	6.214
	9	5.303	0.468	5.964	3.926	1.264	1.433
	10	5.573	1.705	2.638	2.621	1.299	5.549
	11	6.131	1.112	4.793	5.737	2.345	1.174
	12	5.804	2.331	0.053	4.950	2.557	3.473

20	1	5.728	1.435	1.581	5.117	1.929	4.635
	2	5.952	2.396	1.771	4.076	2.311	5.433
	3	5.856	0.810	4.870	4.932	2.359	5.572
	4	5.749	2.295	3.456	6.118	2.049	5.054
	5	5.157	0.392	2.524	5.565	1.825	0.173
	6	5.703	1.834	0.454	4.397	1.680	0.877
	7	5.878	1.659	2.706	6.224	1.511	2.041
	8	5.628	1.535	5.668	1.430	1.600	2.751
	9	5.255	2.651	5.876	4.624	0.959	0.158
	10	6.037	1.231	3.567	0.440	1.127	3.945
	11	5.650	1.821	4.537	5.477	1.942	4.803
	12	5.577	0.765	0.449	4.723	0.591	3.568

Table S49. Molecular coordinates for BC_{12} group 2 structures. Structure 7 resulted from the Shi PES and structure 13 resulted from the van de Waal PES.

Structure	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**
7	1	5.064	0.479	2.569	5.806	0.834	5.448
	2	5.224	2.310	3.290	4.751	2.950	6.131
	3	5.764	2.169	1.765	6.253	2.544	3.850
	4	5.082	0.785	0.230	1.064	1.999	3.480
	5	6.112	1.543	2.557	3.108	0.935	3.140
	6	5.784	1.413	3.636	5.499	2.091	0.625
	7	7.726	2.512	4.424	2.766	2.533	4.682
	8	5.785	1.783	4.634	2.597	0.416	1.981
	9	7.732	2.853	2.205	1.430	0.233	5.655
	10	5.842	1.350	1.573	1.116	2.446	3.942
	11	4.487	2.563	6.050	4.563	2.795	5.973
	12	5.365	0.928	4.879	5.433	3.006	4.863
13	1	5.264	2.166	2.760	2.572	0.701	5.550
	2	5.707	0.562	3.700	6.151	2.192	3.238
	3	6.634	1.166	2.810	3.048	2.302	2.085
	4	5.614	0.858	1.710	3.240	1.904	3.762
	5	5.971	1.450	0.472	2.960	1.678	1.005
	6	5.238	2.479	0.748	1.438	2.652	4.047
	7	5.371	0.661	5.972	1.676	2.701	0.231
	8	5.891	1.723	5.701	2.161	1.588	6.214
	9	6.428	1.255	4.764	1.632	1.965	5.241
	10	5.033	2.440	4.721	1.081	0.610	0.902
	11	6.118	1.536	3.815	1.445	1.480	0.384
	12	8.520	0.100	1.162	4.510	2.947	3.915

Table S50. Molecular coordinates for BC_{12} Group 3, resulting from a calculation on the Shi PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
9	1	5.479	2.200	5.941	4.551	2.870	1.523
	2	6.013	1.559	2.673	4.940	2.126	3.185
	3	5.943	1.694	0.797	2.700	1.385	3.069
	4	5.572	1.685	4.932	2.155	1.694	4.560
	5	7.930	0.024	1.492	4.931	3.089	5.222
	6	5.345	0.701	2.588	3.821	2.509	3.278
	7	5.690	0.697	0.703	3.663	0.808	3.331
	8	4.437	2.606	1.913	2.398	0.255	4.982
	9	8.646	0.761	5.895	5.311	2.271	2.607
	10	5.862	1.354	5.955	1.682	0.460	5.250
	11	5.319	0.658	4.741	1.663	2.475	5.205
	12	6.001	1.375	1.698	0.274	2.053	1.380

Table S51. Molecular coordinates of BC_{12} Group 4 structures. Structures 3, 4, and 5 were calculated on the Jorgenson PES and Structure 8 was calculated on the Shi PES.

Structure	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ
3	1	5.422	1.197	1.632	0.957	1.188	1.218
	2	6.286	1.943	2.157	3.754	0.563	0.899
	3	5.563	2.219	1.027	5.720	1.249	3.589
	4	4.964	3.037	3.118	2.675	1.487	4.074
	5	6.570	1.282	2.812	3.372	2.838	2.144
	6	5.861	2.160	4.306	2.211	1.258	1.710
	7	9.982	1.747	2.641	0.848	1.699	2.930
	8	6.329	1.325	3.898	0.904	2.921	5.236
	9	4.529	0.362	3.015	2.113	0.427	4.949
	10	9.335	2.360	2.443	1.355	2.521	4.009
	11	9.032	2.488	3.342	1.819	0.676	0.973
	12	6.343	1.969	3.204	4.619	0.298	1.310
4	1	6.176	1.960	5.967	4.304	0.579	4.910
	2	6.219	1.867	1.525	1.605	0.973	2.182
	3	7.953	0.391	0.617	1.562	2.973	5.303
	4	5.854	0.977	1.268	5.684	0.427	4.466
	5	6.153	1.076	0.012	5.391	2.374	1.646
	6	4.177	2.878	1.099	3.170	3.083	1.165
	7	9.319	1.468	5.674	2.502	1.342	6.181
	8	4.259	0.292	4.128	4.275	3.096	4.011
	9	6.383	1.714	0.672	3.810	1.692	5.599
	10	5.313	1.328	2.446	5.909	1.927	5.881
	11	5.565	1.411	5.157	0.982	1.237	5.070
	12	8.548	0.823	5.639	6.227	2.841	1.490

5	1	5.700	2.010	3.509	2.734	1.506	4.233
	2	8.264	0.875	1.376	1.947	2.921	3.710
	3	8.219	2.734	0.596	2.214	0.179	4.362
	4	5.941	2.137	1.110	2.880	0.606	2.730
	5	5.888	1.426	1.789	3.084	2.081	4.212
	6	4.887	2.924	4.360	6.184	2.242	0.373
	7	6.232	1.240	2.726	1.753	0.985	0.065
	8	9.333	1.483	1.218	0.353	1.226	4.535
	9	5.901	1.286	0.654	3.879	2.801	3.059
	10	5.990	2.105	2.408	1.807	2.811	5.720
	11	4.147	0.231	2.600	0.828	3.115	5.305
	12	5.418	2.109	6.144	1.963	1.439	2.839
8	1	7.988	0.709	6.094	4.325	0.654	0.556
	2	5.586	1.044	3.972	3.337	0.337	5.494
	3	5.877	1.392	0.241	4.751	2.526	4.037
	4	4.372	0.403	1.552	5.783	3.080	5.002
	5	4.428	3.106	0.916	5.388	2.504	3.225
	6	5.958	1.891	4.672	4.768	1.482	2.751
	7	8.711	1.636	5.157	0.978	1.531	5.484
	8	5.711	1.942	5.884	4.419	0.527	1.602
	9	7.679	0.375	4.357	4.509	3.065	5.987
	10	5.801	2.008	3.781	5.989	1.442	6.197
	11	5.678	1.257	2.862	3.844	1.752	2.399
	12	5.758	0.995	5.346	2.526	2.581	3.948

Table S52. Molecular coordinates of BC_{12} Group 5 structures. Structure 2 came from the Jorgenson PES; structure 10 from Shi; structures 12 and 15 were from van de Waal; 16 and 18 were from the Williams PES.

Structure	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**
2	1	4.272	0.290	3.963	1.042	3.042	4.979
	2	6.041	2.061	3.261	5.347	0.462	2.653
	3	5.927	1.342	2.572	4.122	0.497	3.464
	4	4.249	2.996	6.060	2.568	0.130	1.117
	5	5.910	1.856	4.402	5.678	2.223	5.488
	6	5.920	1.923	2.000	5.369	2.731	1.029
	7	5.848	1.015	1.554	1.812	1.334	0.424
	8	8.984	3.129	2.476	0.037	0.411	2.874
	9	6.362	1.328	3.740	2.039	3.088	5.378
	10	8.334	2.469	2.427	5.477	2.983	4.205
	11	8.362	2.507	3.783	4.836	2.815	5.713
	12	8.198	0.867	3.119	2.107	2.139	6.132

10	1	5.832	1.520	0.345	3.287	1.607	1.043
	2	5.432	0.697	3.981	4.318	0.904	1.791
	3	5.507	0.892	5.726	5.761	0.317	2.937
	4	6.110	1.708	5.681	4.320	0.358	2.101
	5	4.867	2.475	4.354	2.568	0.395	3.451
	6	5.967	1.458	4.612	0.373	1.686	1.875
	7	4.982	2.418	0.991	4.869	2.769	3.475
	8	7.773	3.135	2.430	5.684	0.449	5.169
	9	8.757	1.992	5.132	0.732	0.847	1.505
	10	9.444	1.373	5.216	1.394	2.243	1.691
	11	7.739	2.484	5.802	3.544	1.265	5.432
	12	4.703	0.460	1.537	0.036	0.975	1.738
12	1	6.266	2.098	4.080	2.035	2.635	0.131
	2	4.525	2.888	0.581	2.085	0.588	2.332
	3	6.459	1.332	4.614	0.916	0.034	5.476
	4	5.577	1.036	2.486	4.985	0.721	1.769
	5	9.363	1.868	3.428	0.503	1.695	3.142
	6	4.818	0.376	4.907	2.146	0.634	1.589
	7	6.386	1.254	3.601	5.704	1.849	2.373
	8	5.574	2.032	2.766	1.772	2.277	3.067
	9	8.486	2.536	4.853	6.101	2.821	1.922
	10	6.500	1.909	5.225	1.909	0.564	3.538
	11	9.653	3.119	0.682	3.154	2.667	1.209
	12	8.898	2.536	3.403	3.628	2.864	1.495
15	1	8.692	0.662	5.667	3.828	0.505	3.029
	2	9.054	1.175	6.248	2.463	2.128	3.364
	3	8.849	0.134	0.932	1.287	0.305	2.141
	4	5.894	2.400	3.981	5.975	2.210	1.077
	5	8.657	2.742	5.252	4.919	0.420	2.039
	6	5.391	0.509	4.311	1.406	1.945	3.488
	7	4.957	2.762	1.522	2.924	2.171	1.878
	8	6.044	1.329	5.623	0.769	2.602	3.071
	9	5.384	0.693	0.687	0.058	0.321	4.247
	10	5.627	2.206	5.693	4.027	2.883	3.623
	11	6.116	1.511	4.605	1.893	1.239	1.340
	12	5.811	1.679	0.509	6.160	1.255	3.797
16	1	5.638	2.457	1.078	5.433	1.922	2.743
	2	5.836	2.395	5.716	3.734	0.729	4.994
	3	5.571	1.336	3.764	4.688	1.976	0.166
	4	6.303	1.910	4.591	3.461	3.026	2.729
	5	6.626	1.181	4.852	0.523	0.240	1.769
	6	4.394	0.184	5.333	5.747	2.881	4.441
	7	7.983	2.459	2.192	0.902	1.506	5.343
	8	8.676	3.120	0.901	2.964	2.420	4.266
	9	8.312	1.690	5.389	1.567	1.970	5.403
	10	5.889	1.324	5.992	5.991	1.809	5.576
	11	5.142	2.445	3.455	3.819	2.736	1.778
	12	9.259	2.424	4.602	2.070	0.345	1.053

18	1	4.266	3.098	0.358	5.135	2.979	5.553
	2	4.258	0.208	3.882	1.182	3.109	3.300
	3	5.473	1.228	0.604	2.599	2.116	3.262
	4	10.071	1.740	2.897	1.031	1.694	3.292
	5	5.896	1.233	1.694	1.423	2.297	5.628
	6	5.782	1.833	3.486	4.070	0.730	1.166
	7	8.936	2.446	1.708	3.934	0.247	0.467
	8	9.086	3.067	3.437	2.949	2.993	0.726
	9	6.419	1.970	1.237	5.387	0.206	0.796
	10	8.713	2.392	2.897	0.465	2.757	4.168
	11	6.499	1.968	2.371	3.125	2.746	4.028
	12	6.678	1.230	2.836	0.243	0.377	0.608

Table S53. Molecular coordinates of BC_{12} Group 6, calculated on the Williams PES.

Structure	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**
17	1	9.232	2.524	5.084	2.614	1.796	4.040
	2	11.935	2.438	5.855	4.266	0.570	2.965
	3	4.602	0.322	0.518	5.134	2.466	4.898
	4	4.648	2.769	3.931	4.924	2.738	5.716
	5	9.305	2.151	4.346	4.452	2.331	3.621
	6	6.620	1.854	4.881	2.632	2.766	2.590
	7	5.554	1.019	4.490	1.409	3.081	0.950
	8	5.557	1.354	5.693	1.462	1.223	6.085
	9	5.666	2.093	0.404	2.386	0.083	0.135
	10	8.486	2.090	5.760	1.812	2.852	5.117
	11	6.473	1.761	3.810	4.238	2.890	5.182
	12	8.006	2.760	0.235	0.641	0.276	2.143

Table S54. Deviations of BC_{12} structures from model icosahedron. Distances are in angstroms and angles are in degrees.

		Distance			Angle	
Group	Structure	CM-to-molecule (Std. Dev.)	Inner (Std. Dev.)	Outer (Std. Dev.)	Inner (Std. Dev.)	Outer (Std. Dev.)
1	1	0.3	0.4	1.1	14	17
	6	0.4	0.5	1.1	17	20
	11	0.3	0.3	1.3	14	17
	14	0.2	0.2	1.3	15	18
	19	0.3	0.3	1.2	14	16
	20	0.2	0.3	1.3	20	22
2	7	0.9	1.0	1.0	9	12
	13	0.8	0.9	1.0	15	18
3	9	1.1	1.1	1.0	16	19
4	3	1.3	1.7	1.1	14	16
	4	1.4	1.5	1.0	15	17
	5	1.4	1.5	1.0	18	20
	8	1.2	1.3	1.0	15	17
5	2	1.5	1.5	1.0	18	19
	10	1.4	1.5	0.9	18	20
	12	1.5	1.7	1.0	18	20
	15	1.6	1.5	1.0	19	21
	16	1.5	1.5	0.8	13	15
	18	1.5	1.9	1.0	17	20
6	17	1.6	2.1	0.9	12	15

Table S55. Benzene energy (Ben. E.) and cluster energy (Cluster E.) values and ratios, and the ratio of benzene to total cluster stabilization are shown for all BC_{12} structures. The last column identifies the relevant PES.

Group	Structure	Ben. E. (kJ/mol)	Ben. E Ratio (%)	Cluster E. (kJ/mol)	Cluster E. Ratio (%)	E_B / E_{tot} Ratio (%)	PES
1	1	-42.58	100.0	-330.58	100.0	12.9	Jorgensen
	6	-38.20	100.0	-278.64	100.0	13.7	Shi
	11	-39.76	98.4	-286.15	99.3	13.9	van de Waal
	14	-40.39	100.0	-288.19	100.0	14.0	van de Waal
	19	-39.52	99.1	-291.84	100.0	13.5	Williams
	20	-39.87	100.0	-291.70	100.0	13.7	Williams
2	7	-34.96	91.5	-268.70	96.4	13.0	Shi
	13	-36.38	90.1	-273.54	94.9	13.3	van de Waal
3	9	-34.17	89.5	-268.78	96.5	12.7	Shi
4	3	-30.51	71.6	-316.27	95.7	9.6	Jorgensen
	4	-33.40	78.4	-315.36	95.4	10.6	Jorgensen
	5	-33.56	78.8	-311.50	94.2	10.8	Jorgensen
	8	-32.83	85.9	-264.07	94.8	12.4	Shi
5	2	-31.02	72.8	-305.40	92.4	10.2	Jorgensen
	10	-29.19	76.4	-263.96	94.7	11.1	Shi
	12	-28.66	71.0	-270.85	94.0	10.6	van de Waal
	15	-28.96	71.7	-264.68	91.8	10.9	van de Waal
	16	-28.96	72.6	-267.52	91.7	10.8	Williams
	18	-28.49	71.5	-270.02	92.5	10.6	Williams
6	17	-26.48	66.4	-264.43	90.6	10.0	Williams

S. G. Structures and Energies of Individual BC_n Isomers: BC_3 Minor Isomers

Tables S56-S61 document the mean molecular coordinates for the six *minor* **BC_3** isomers, 6-11, resulting from the MC simulations. Also tabulated for each PES are the corresponding molecular coordinates, the optimized energies, and the mean-square displacement of the PES's atomic coordinates relative to the mean structure's coordinates. **Figures S1-S2** illustrate the structures from the z and x axis, respectively.

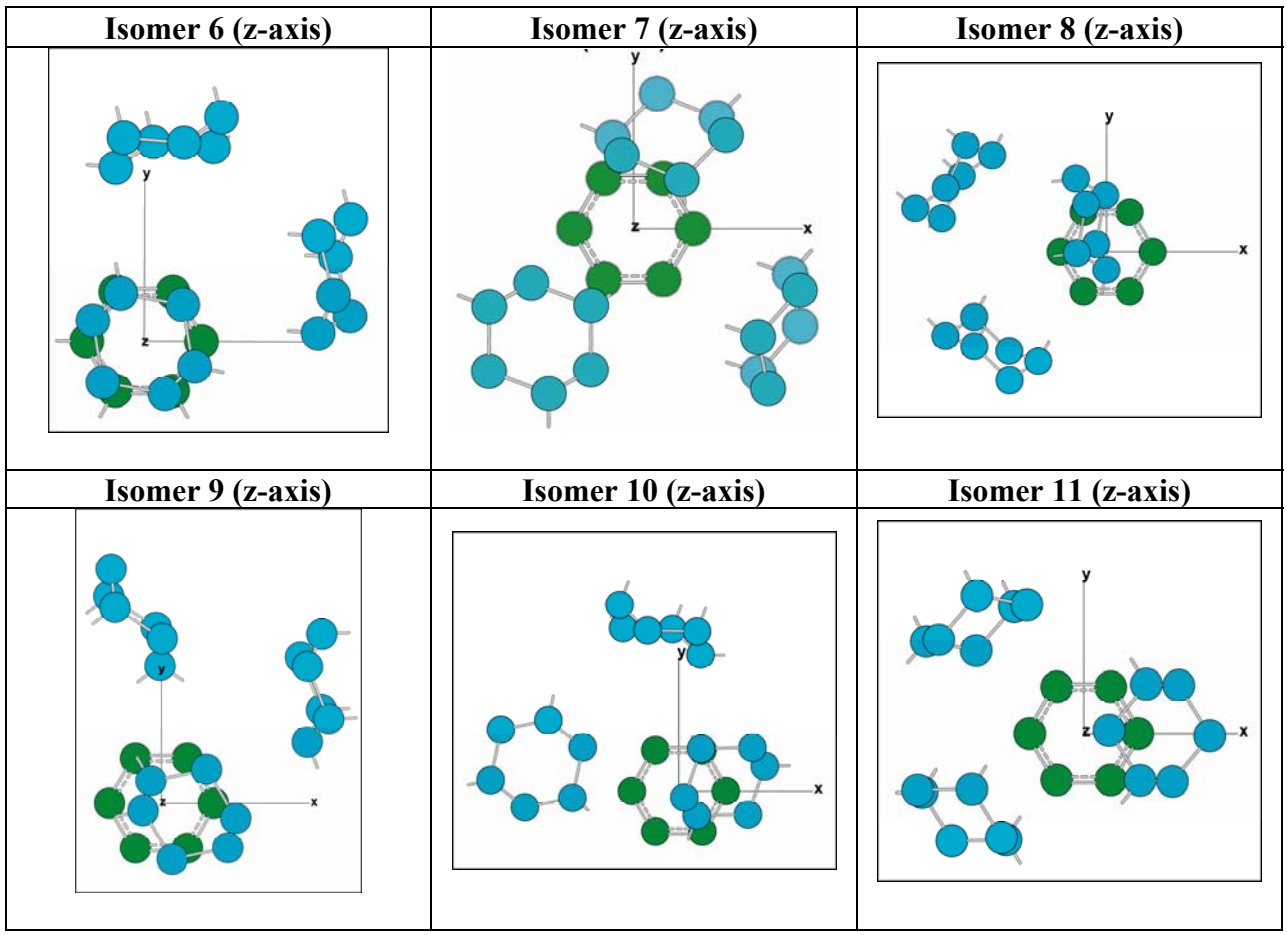

Figure S1. BC_3 *minor* isomers, viewed from the +z axis. The carbon atoms in the benzene molecule are green and the cyclohexane carbons are blue. Hydrogen atoms are not shown

Table S56. Molecular coordinates for Isomer 6, based on the Shi and Williams PESs only, along with optimized energy and mean-square displacement values for each PES.

Isomer 6	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ	E (kJ mol^{-1})	<(Δr)^2>
Shi (3)	1	5.569	1.095	1.451	4.977	1.448	4.953	-48.05	0.018
	2	4.346	0.004	3.530	2.105	0.550	3.911		
	3	5.544	1.098	0.340	3.462	1.394	6.221		
van de Waal	1	5.789	1.076	1.470	5.006	1.473	4.944	-48.90	0.018
	2	4.504	0.044	3.783	2.087	0.573	3.932		
	3	5.774	1.073	0.331	3.493	1.376	6.225		
Mean	1	5.679	1.085	1.461	4.992	1.461	4.948		
	2	4.425	0.024	3.657	2.096	0.561	3.922		
	3	5.659	1.085	0.336	3.477	1.385	6.223		
Standard Deviation	1	0.155	0.014	0.013	0.020	0.018	0.006		
	2	0.111	0.028	0.180	0.013	0.016	0.015		
	3	0.163	0.018	0.007	0.022	0.013	0.002		

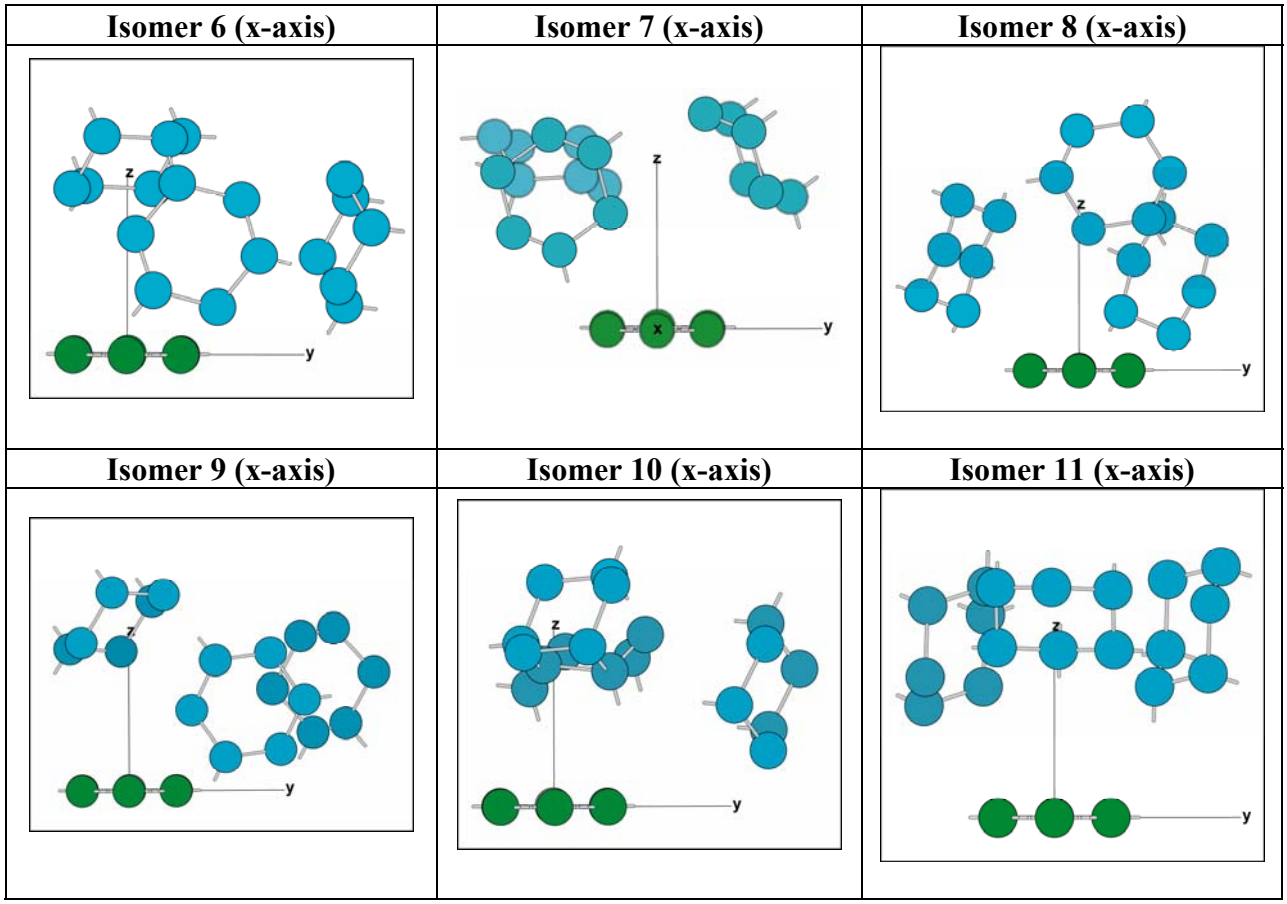

Figure S2. View of each BC_3 *minor* isomer from the +x axis. The carbon atoms in the benzene molecule are green and the cyclohexane carbons are blue. The hydrogen atoms are omitted

Table S57. Molecular coordinates for Isomer 7, based on the Shi, van de Waal, and Williams PESs, along with optimized energy and mean-square displacement values for each PES.

Isomer 7	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ	E (kJ mol^{-1})	$\langle(\Delta r)^2\rangle$
Shi (3)	1	4.694	0.476	1.172	0.106	0.916	1.706	-47.90	0.050
	2	5.183	0.737	4.051	1.203	2.774	3.892		
	3	5.334	0.912	5.636	0.225	1.472	5.959		
van de Waal	1	4.936	0.515	1.250	0.097	0.957	1.714	-48.81	0.016
	2	5.359	0.713	3.993	1.321	2.736	3.987		
	3	5.515	0.876	5.663	0.183	1.433	5.953		
Williams	1	4.921	0.540	1.200	0.128	0.957	1.672	-49.15	0.025
	2	5.254	0.679	3.993	1.237	2.705	3.902		
	3	5.474	0.880	5.684	0.185	1.447	5.941		
Mean	1	4.850	0.510	1.207	0.110	0.943	1.697		
	2	5.265	0.710	4.012	1.254	2.738	3.927		
	3	5.441	0.889	5.661	0.198	1.451	5.951		
Standard Deviation	1	0.135	0.032	0.039	0.016	0.024	0.022		
	2	0.089	0.029	0.034	0.060	0.035	0.052		
	3	0.095	0.020	0.024	0.024	0.020	0.009		

Table S58. Molecular coordinates for Isomer 8, based on the Shi, van de Waal, and Williams PESs, along with optimized energy and mean-square displacement values for each PES.

Isomer 8	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ	E (kJ mol^{-1})	$\langle(\Delta r)^2\rangle$
Shi (3)	1	5.628	1.996	5.852	6.078	1.793	2.425	-47.93	0.034
	2	4.946	2.944	5.222	2.698	1.324	0.131		
	3	5.380	2.126	0.700	0.354	1.893	1.082		
van de Waal	1	5.860	2.007	5.843	6.087	1.768	2.404	-48.9	0.013
	2	5.108	2.962	5.102	2.704	1.350	0.121		
	3	5.625	2.137	0.705	0.374	1.892	1.076		
Williams	1	5.746	2.052	5.836	6.121	1.721	2.448	-49.07	0.034
	2	5.085	2.970	4.908	2.712	1.406	0.097		
	3	5.537	2.161	0.730	0.415	1.900	1.107		
Mean	1	5.745	2.018	5.844	6.095	1.761	2.426		
	2	5.046	2.959	5.077	2.704	1.360	0.116		
	3	5.514	2.142	0.712	0.381	1.895	1.088		
Standard Deviation	1	0.116	0.030	0.008	0.022	0.037	0.022		
	2	0.088	0.013	0.158	0.007	0.042	0.018		
	3	0.124	0.018	0.016	0.031	0.005	0.016		

Table S59. Molecular coordinates for Isomer 9, based on all four PESs, along with optimized energy and mean-square displacement values for each PES.

Isomer 9	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**	**E (kJ mol^{-1})**	**<(Δr)^2>**
Jorgensen	1	4.459	0.167	6.319	0.956	2.508	1.027	-54.48	0.095
	2	5.661	1.198	0.648	3.603	1.475	3.159		
	3	5.880	1.108	1.674	3.558	1.498	3.755		
Shi (3)	1	4.444	0.184	5.902	0.891	2.466	1.032	-47.37	0.029
	2	5.639	1.161	0.645	3.561	1.499	3.189		
	3	5.801	1.061	1.709	3.528	1.591	3.784		
van de Waal	1	4.712	0.137	5.622	0.667	2.336	0.863	-47.88	0.119
	2	5.850	1.096	0.611	3.469	1.566	3.127		
	3	6.080	1.054	1.703	3.528	1.620	3.688		
Williams	1	4.547	0.151	5.866	0.935	2.472	1.038	-48.48	0.011
	2	5.798	1.146	0.636	3.548	1.519	3.223		
	3	6.042	1.070	1.696	3.530	1.572	3.702		
Mean	1	4.540	0.160	5.927	0.862	2.445	0.990		
	2	5.737	1.150	0.635	3.545	1.515	3.175		
	3	5.951	1.073	1.696	3.536	1.570	3.732		
Standard Deviation	1	0.123	0.020	0.289	0.133	0.076	0.085		
	2	0.103	0.042	0.017	0.056	0.039	0.041		
	3	0.132	0.024	0.016	0.015	0.052	0.045		

Table S60. Molecular coordinates for Isomer 10, based on all four PESs, along with optimized energy and mean-square displacement values for each PES.

Isomer 10	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**	**E (kJ mol^{-1})**	**<(Δr)^2>**
Jorgensen	1	4.574	2.896	3.606	6.308	0.746	5.292	-54.31	0.355
	2	5.491	2.130	6.034	3.212	0.210	4.392		
	3	5.590	2.025	4.850	1.359	1.468	4.307		
Shi (3)	1	4.576	2.833	3.341	6.258	0.789	5.360	-47.37	0.025
	2	5.404	2.215	6.094	2.713	0.269	4.915		
	3	5.553	2.077	4.828	1.284	1.493	4.359		
van de Waal	1	4.827	2.754	3.143	6.200	0.860	5.409	-48.05	0.154
	2	5.501	2.302	6.151	2.504	0.351	5.144		
	3	5.740	2.132	4.781	1.194	1.527	4.382		
Williams	1	4.779	2.755	3.197	6.176	0.841	5.448	-48.46	0.138
	2	5.459	2.312	6.151	2.414	0.364	5.239		
	3	5.691	2.125	4.791	1.208	1.515	4.405		
Mean	1	4.689	2.809	3.321	6.236	0.809	5.377		
	2	5.464	2.240	6.108	2.711	0.298	4.922		
	3	5.644	2.090	4.813	1.261	1.501	4.363		
Standard Deviation	1	0.133	0.068	0.207	0.059	0.052	0.068		
	2	0.044	0.085	0.056	0.357	0.072	0.379		
	3	0.087	0.050	0.032	0.076	0.026	0.042		

Table S61. Molecular coordinates for Isomer 11, based on all four PESs, along with optimized energy and mean-square displacement values for each PES.

Isomer 11	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**	**E (kJ mol^{-1})**	**$\langle(\Delta r)^2\rangle$**
Jorgensen	1	4.698	2.748	3.165	3.117	2.475	6.207	-53.48	0.018
	2	5.733	2.346	5.517	4.007	1.282	5.161		
	3	5.305	2.314	0.582	0.119	1.253	4.149		
Shi (3)	1	4.706	2.711	3.149	3.109	2.489	6.192	-46.74	0.016
	2	5.720	2.369	5.484	3.972	1.289	5.152		
	3	5.296	2.338	0.592	0.088	1.240	4.166		
van de Waal	1	4.857	2.720	3.157	3.120	2.497	6.215	-47.60	0.018
	2	5.957	2.355	5.505	3.992	1.292	5.177		
	3	5.531	2.322	0.607	0.091	1.255	4.165		
Williams	1	4.842	2.730	3.123	3.138	2.465	6.194	-48.22	0.012
	2	5.911	2.361	5.473	3.990	1.287	5.121		
	3	5.463	2.326	0.564	0.090	1.257	4.150		
Mean	1	4.776	2.727	3.149	3.121	2.481	6.202		
	2	5.830	2.358	5.495	3.991	1.288	5.153		
	3	5.399	2.325	0.586	0.097	1.251	4.157		
Standard Deviation	1	0.085	0.016	0.018	0.012	0.014	0.011		
	2	0.122	0.010	0.020	0.014	0.004	0.024		
	3	0.117	0.010	0.018	0.015	0.008	0.009		

S. H. Structures and Energies of Individual BC_n Isomers: BC_3 Hypothetical Isomers

Tables S62-S64 document the mean molecular coordinates for the three *hypothetical* **BC_3** isomers, H1-H3, *not* predicted by the MC simulations. Also tabulated for each PES are the corresponding molecular coordinates, the optimized energies, and the mean-square displacement of the PES's atomic coordinates relative to the mean structure's coordinates. **Figure S3** illustrates the structures from the perspective of the z and x axes.

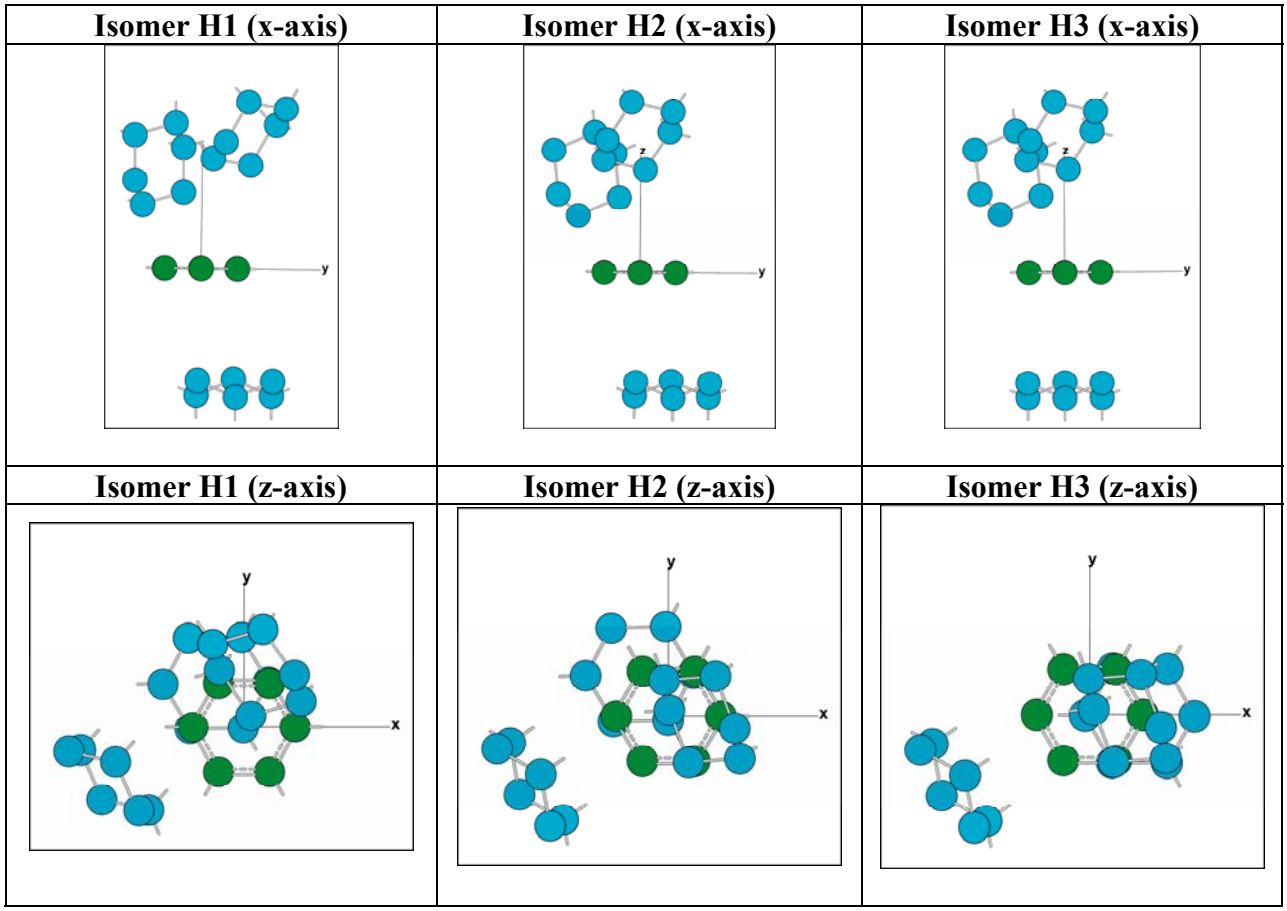

Figure S3. View of three BC_3 *hypothetical* isomers from the +x axis (top) and +z axis (bottom). The carbon atoms in the benzene molecule are green and the cyclohexane carbons are blue. The hydrogen atoms are omitted.

Table S62. Molecular coordinates for *hypothetical* Isomer H1, based on all four PESs, along with optimized energy and mean-square displacement values for each PES. Standard deviations marked with an asterisk are not meaningful because β is near zero, in which case α and γ are mutually dependent, and only the sum, α + γ, is independent.

Isomer H1	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**	**E (kJ mol^{-1})**	**$\langle(\Delta r)^2\rangle$**
Jorgensen	1	4.803	0.285	1.311	0.431	0.895	4.028	-42.38	0.021
	2	5.287	0.873	3.522	0.883	1.728	0.783		
	3	4.222	2.803	2.171	3.552	0.034	-0.390		
Shi (3)	1	4.795	0.342	1.349	0.417	0.856	4.071	-38.08	0.019
	2	5.276	0.852	3.506	0.889	1.761	0.821		
	3	4.226	2.803	2.157	3.085	0.022	0.075		
van de Waal	1	4.955	0.319	1.271	0.436	0.872	4.033	-39.52	0.016
	2	5.514	0.859	3.526	0.905	1.762	0.864		
	3	4.376	2.845	2.163	2.281	0.018	0.877		
Williams	1	4.895	0.319	1.218	0.385	0.848	4.069	-39.58	0.013
	2	5.450	0.843	3.527	0.917	1.764	0.826		
	3	4.323	2.847	2.171	2.110	0.021	1.050		
Mean	1	4.861	0.316	1.287	0.417	0.868	4.050		
	2	5.381	0.857	3.521	0.898	1.754	0.823		
	3	4.286	2.825	2.165	2.890	0.020	0.270		
Standard Deviation	1	0.077	0.023	0.056	0.023	0.021	0.023		
	2	0.118	0.012	0.010	0.016	0.017	0.033		
	3	0.076	0.025	0.007	0.7*	0.007	0.7*		

Table S63. Molecular coordinates for *hypothetical* Isomer H2, based on all four PESs, along with optimized energy and mean-square displacement values for each PES. . Results from an independent MP2 electronic structure optimization are shown in the bottom three rows. Standard deviations marked with an asterisk are not meaningful because β is near zero, in which case α and γ are mutually dependent; only the sum, α + γ, is independent. MP2 result was a better fit to H1, with $\langle(\Delta r)^2\rangle = 1.5$.

Isomer H2	**C_6H_{12}**	**R (Å)**	**Θ**	**Φ**	**α**	**β**	**γ**	**E (kJ mol^{-1})**	**$\langle(\Delta r)^2\rangle$**
Jorgensen	1	4.756	0.175	6.134	0.518	0.915	3.762	-42.52	0.026
	2	5.314	0.910	3.600	0.994	1.648	0.601		
	3	4.219	2.812	2.186	3.416	0.031	-0.248		
Shi (3)	1	4.747	0.191	6.187	0.542	0.910	3.753	-38.01	0.014
	2	5.308	0.895	3.603	1.003	1.663	0.596		
	3	4.224	2.812	2.172	2.747	0.023	0.419		
van de Waal	1	4.935	0.216	6.459	0.526	0.914	3.761	-39.41	0.032
	2	5.497	0.870	3.580	0.970	1.713	0.662		
	3	4.373	2.854	2.163	1.790	0.018	1.375		
Williams	1	4.880	0.212	6.470	0.513	0.903	3.794	-39.51	0.024
	2	5.444	0.865	3.584	0.981	1.708	0.639		
	3	4.320	2.856	2.180	2.036	0.026	1.127		
Mean	1	4.827	0.196	6.283	0.525	0.911	3.767		
	2	5.390	0.884	3.592	0.986	1.683	0.625		
	3	4.283	2.834	2.175	2.595	0.019	0.571		
Standard Deviation	1	0.093	0.019	0.177	0.012	0.006	0.018		
	2	0.095	0.021	0.012	0.015	0.032	0.032		
	3	0.075	0.025	0.010	0.7*	0.006	0.7*		
MP2/6-31g(d)	1	4.624	0.359	1.056	3.167	0.759	5.140		2.2*
	2	5.291	0.830	3.570	2.427	1.596	0.214		
	3	4.137	2.851	2.134	1.961	0.054	1.161		

Table S64. Molecular coordinates for *hypothetical* Isomer H3, based on all four PESs, along with optimized energy and mean-square displacement values for each PES. Standard deviations marked with an asterisk are not meaningful because β is near zero, in which case α and γ are mutually dependent; only the sum, α + γ, is independent.

Isomer H3	C_6H_{12}	R (Å)	Θ	Φ	α	β	γ	E (kJ mol^{-1})	$\langle(\Delta r)^2\rangle$
Jorgensen	1	4.764	0.195	6.179	0.510	0.904	3.780	-42.32	0.023
	2	5.296	0.890	3.619	1.001	1.665	0.613		
	3	4.215	2.825	6.264	4.463	0.014	2.861		
Shi (3)	1	4.759	0.212	6.187	0.531	0.903	3.767	-37.85	0.016
	2	5.293	0.878	3.623	1.014	1.675	0.601		
	3	4.222	2.823	6.262	0.394	0.006	0.646		
van de Waal	1	4.954	0.242	0.133	0.518	0.904	3.762	-39.27	0.031
	2	5.473	0.849	3.593	0.979	1.731	0.661		
	3	4.371	2.864	6.259	0.623	0.018	0.422		
Williams	1	4.894	0.233	0.138	0.507	0.894	3.802	-39.38	0.020
	2	5.430	0.848	3.606	0.995	1.720	0.642		
	3	4.315	2.872	6.269	1.057	0.024	-0.017		
Mean	1	4.840	0.219	6.283	0.516	0.901	3.777		
	2	5.372	0.866	3.610	0.997	1.697	0.629		
	3	4.280	2.846	6.263	0.615	0.009	0.427		
Standard Deviation	1	0.097	0.021	3.492	0.011	0.005	0.018		
	2	0.092	0.021	0.013	0.015	0.032	0.028		
	3	0.075	0.026	0.004	1.9*	0.008	1.3*		

Tables S65-S66 demonstrate uniqueness of the BC_3 isomers, and identify structures that retain their identities in isothermal simulations at 5 K.

Table S65. Uniqueness of mean optimized isomers: mean squared atomic displacement, $\langle(\Delta r)^2\rangle$. A value of zero (diagonal entries) indicates that the structures are identical.

$\langle(\Delta r)^2\rangle$	1	2	3	4	5	6	7	8	9	10	11	H1	H2	H3
1	**0.0**	25	1.9	7.2	0.9	0.6	7.6	1.2	2.0	3.1	6.7	23	24	28
2		**0.0**	27	37	26	27	36	28	27	31	38	11	10	11
3			**0.0**	6.7	1.7	0.6	8.6	2.8	2.9	4.7	5.5	22	22	26
4				**0.0**	8.4	5.5	2.9	5.7	8.1	4.8	1.6	26	25	27
5					**0.0**	1.4	9.0	2.1	1.5	3.6	7.3	24	24	29
6						**0.0**	6.5	1.3	2.0	2.9	4.9	24	23	27
7							**0.0**	6.5	7.4	2.7	4.7	29	27	30
8								**0.0**	2.6	2.9	5.4	24	24	28
9									**0.0**	2.7	7.3	25	25	29
10										**0.0**	5.3	27	25	28
11											**0.0**	28	27	29
H1												**0.0**	0.9	2.7
H2													**0.0**	1.7
H3														**0.0**

Table S66. Isothermal runs on Shi PES at 5 K to determine uniqueness of isomers. The initial isomer structure is indicated by the row headings, and the final structure by column headings. Entries indicate the mean square atomic displacement of the final structures relative to the standard (initial) structures. At 5 K, Isomer 6 was transformed to Isomer 3, and H2 was transformed to H1, indicating shallow barriers to interconversion between the respective structures. All other isomers retained their original structures.

5K	1	2	3	4	5	6	7	8	9	10	11	H1	H2	H3
1	0.01													
2		0.04												
3			0.02											
4				0.01										
5					0.01									
6			0.02			~~0.71~~								
7							0.02							
8								0.04						
9									0.03					
10										0.03				
11											0.02			
H1												0.01		
H2												0.03	~~1.22~~	
H3														0.01

S I. Structural Grouping, Properties, and Energies of BC_n Cluster Groups: BC_5

S. *I. A. BC_5 Group 1.* The structures of Group 1 have cyclohexanes located on both sides of the x, y-plane but only on one half of the benzene hexagon, forming a partial shell around the benzene (**Figure 7**). A horizontally oriented cap molecule is present on both sides of the plane; the two caps are not precisely parallel to one another. The other cyclohexanes are distributed nearly evenly in the half-shell formation. Group 1 is subdivided into three subgroups (1A, 1B and 1C). Molecular coordinates for the isomers of the three subgroups are documented in **Tables S21-23**. In subgroup 1A, two vertically oriented cyclohexanes ($\beta > 0.9$ radians) have CMs located in or near the x, y plane ($1.37 < \theta <$ 1.77 radians). The remaining 3 cyclohexane molecules are split 2-1 above/below the x-y plane (**Figure 7**).

In subgroup 1B structures, a single, vertically-oriented cyclohexane has its CM positioned in the x, y plane. The remaining four cyclohexanes are evenly split above/below the x, y plane (**Figure 7**). Subgroup 1C structures are similar to those of subgroup 1B, except that the cyclohexane located in the

x, y-plane assumes a horizontal orientation (**Figure 7**). Furthermore, *all* cyclohexane molecules in Group 1C have *horizontal* orientations.

Of the 26 BC_5 simulated structures, 11 (~42%) belong to Group 1. Of these, 5 (~19%) are assigned to subgroup 1A, 5 (~19%) to subgroup 1B, and 1 (~4%) to subgroup 1C.

S. I. B. BC_5 Group 2. The molecular coordinates for the isomers of Group 2 are collected in **Table S24**. In Group 2 structures, four cyclohexane molecules are located on one side of the x, y-plane, with the fifth oriented horizontally ($\beta > 0.9$ radians) on the opposite side (**Figure 7**). The cyclohexanes do not form a half shell around the benzene; instead, three of the four molecules below the plane form a triangular ring that is off-center relative to the z-axis. The fourth cyclohexane is positioned directly under the ring, and assumes a horizontal orientation (**Figure 7**). Of the 26 BC_5 isomers, 3 (~12%) are classified in Group 2.

S. I. C. BC_5 Group 3. Group 3 structures are characterized by a four-molecule formation in which the molecular CMs are nearly coplanar; the planes are represented in **Figure S4** by grey lines. Such planes are expected in a quasi-octahedral structure. In addition to the distance and angle deviation calculations, a 3-D linear fit to the equation of a plane was preformed on the CM coordinates of the four "coplanar" molecules. The resulting regression coefficients (R^2), listed for each Group 3 isomer in **Table S67**, were a factor in subgrouping these structures. The majority of structures have all five cyclohexanes located on the same side of the benzene x, y-plane; the single exception is the structure assigned to subgroup 3A, for which the molecular coordinates are collected in **Table S25**. The cyclohexanes in subgroup 3A form a half shell partially encasing the benzene (**Figure S4**). This half-shell structure is similar to that of Group 1, the key difference being that in 3A the benzene moiety participates in a near-planar four-ring structure. On closer inspection, three different four-molecule planes are observed, meeting expectations for a near-octahedron. The R^2 value from the linear fit is 0.933 for the plane oriented nearly along the y-axis, 0.868 for the plane oriented in the z direction, and 0.354 for the plane oriented along the x-axis, the latter of which is represented by four connected lines in

Figure S4 (see **Table S67**). The first regression coefficient (0.933) is the largest among all Group 3 structures, indicating that the subgroup 3A structure most closely resembles a model octahedron. The remaining structures of Group 3, subgroups 3B-3D, have all five cyclohexane molecules positioned on the same side of the x-y plane; together they encircle the z-axis (**Figure S4**). The four-molecule plane is tilted relative to the cluster plane, more in some structures than in others. Molecular coordinates for isomers identified with subgroups 3B, 3C, and 3D are listed in **Tables S26-28**. The major distinction between the three subgroups lies in the regression coefficients derived from planarity analysis. Subgroup 3B structures have R^2 values that fall in the 0.8 - 0.9 range; subgroup 3C isomers fall in the 0.6 - 0.7 range and subgroup 3D has R^2 values found in the 0.4 to 0.5 range (**Table S67**). The structures become less "octahedral" in the order 3A > 3B > 3C > 3D. Of the 26 BC_5 isomers, 12 (~46%) are members of Group 3. One (~4%) belongs to subgroup 3A, six (~23%) belong to subgroup 3B, two (~8%) are in subgroup 3C, and three (~12%) are classified with subgroup 3D.

Table S67. Regression coefficients (R^2) of each BC_5 Group 3 structure, based on a 3D linear regression to the equation of a plane.

Group	Structure	R^2
3A	14	0.93
3B	1	0.86
	7	0.89
	8	0.83
	10	0.82
	13	0.79
	15	0.84
3C	6	0.63
	16	0.64
3D	9	0.40
	12	0.49
	22	0.43

Table S68. The average Benzene energy ratio (Ben. E. Ratio), Cluster energy ratio (Cluster E. Ratio), distance deviation (Dist. Dev.) and angle deviation (angle Dev.) for each subgroup of BC_5, with the corresponding standard deviation (Std. Dev.).

Group	Ave. Ben E. Ratio (%)	Std. Dev.	Ave. Cluster E. Ratio (%)	Std. Dev.	Ave. Dist. Dev. (%)	Std. Dev. (%)	Ave. Angle Dev. (%)	Std. Dev. (%)
Subgroup 1B	96.8	2.7	98.6	1.1	17.3	0.6	17.5	4.0
Subgroup 1B	97.6	3.1	98.5	1.7	16.0	0.6	27.0	4.4
Subgroup 1C	80.4	--	97.3	--	11.9	--	17.5	--
Group 2	81.3	4.4	96.7	4.1	12.2	0.9	30.1	4.8
Subgroup 3A	95.7	--	99.8	--	16.8	--	7.5	--
Subgroup 3B	68.0	6.7	98.8	1.1	13.2	1.2	10.7	4.5
Subgroup 3C	68.8	7.9	98.2	0.8	14.5	2.8	17.5	4.0
Subgroup 3D	65.0	6.9	99.1	0.8	15.9	2.4	18.1	8.3

S.I.D. Energy and Deviation Comparisons for BC_5 Isomers

BC_5 benzene-molecule and total-cluster stabilization energies were converted to percent ratios as defined earlier. **Table S68** lists the average benzene and cluster energy ratios (with standard deviations) for each BC_5 subgroup. For additional documentation of the benzene-molecule and total-cluster energy ratios for each individual structure, see **Table S29**. The total cluster energy ratios range between 95 - 100% for all subgroups; however, differentiation is observed in the benzene stabilization ratios. Subgroups 1A, 1B, and 3A, in which the cyclohexanes form a partial shell around the benzene moiety, have relatively large benzene stabilization ratios (96-98 %). Subgroups 3B, 3C, and 3D, in which all five cyclohexanes are on the same side of the x, y-plane, have the smallest benzene stabilization, ranging from 65-69%. The benzene stabilization ratios tend to fall into one of three ranges: 65-69%, 80-82%, or 95-98% (**Table S68**).

The relative distance and angle deviations from the model octahedral structure (with standard deviations) are collected in **Table S68** for each subgroup. (For documentation of the deviation results for individual BC_5 structures, see **Table S30**.) The distance deviations are comparable for all subgroups. In contrast, the angle deviations and results of the planarity calculations (**Table S67**) suggest that 3A and 3B structures are relatively similar to the model octahedron.

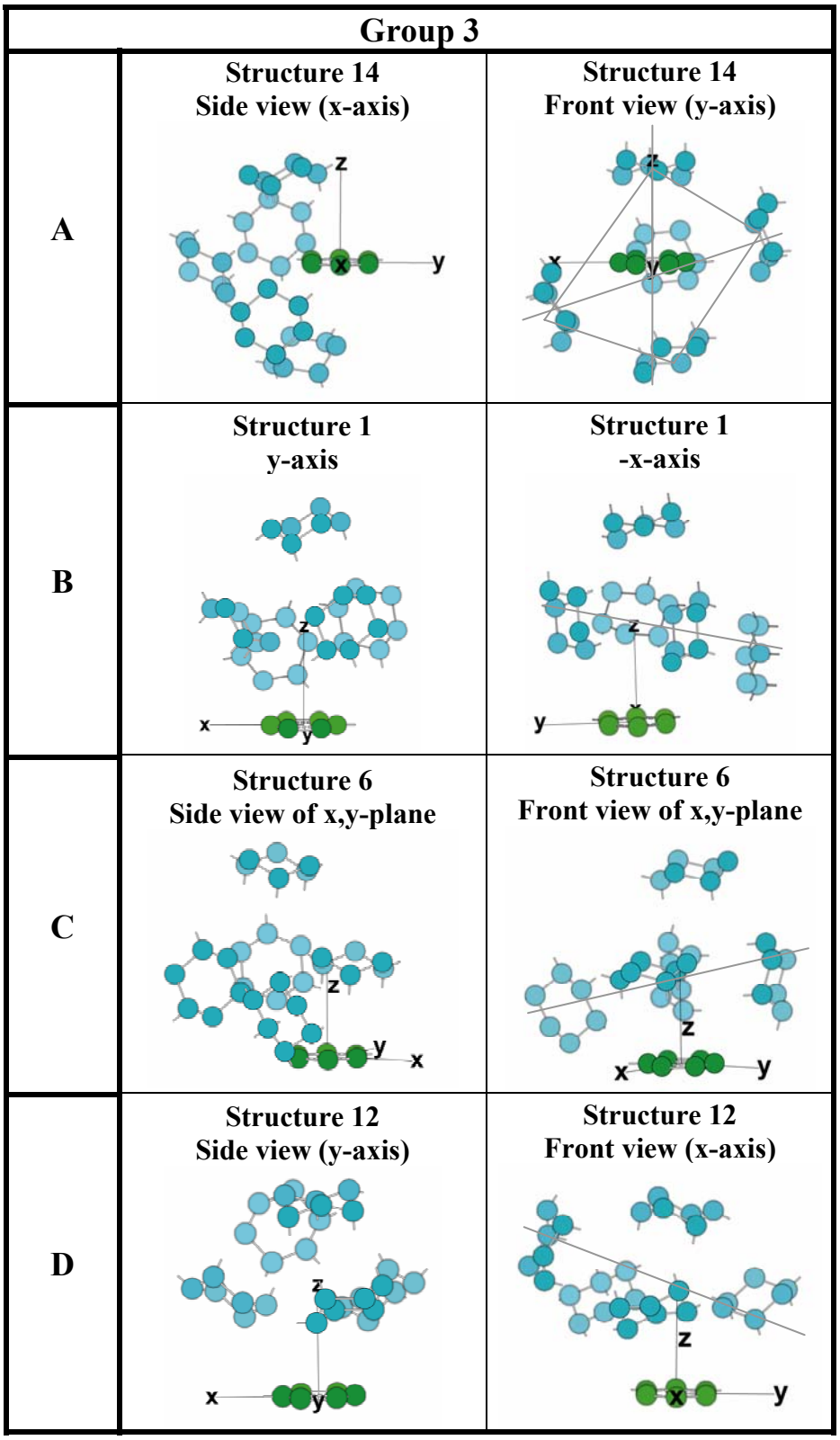

Figure S4. Representative structures for each subgroup of BC_5 Group 3 clusters. Structures are shown from two different views in the x, y-plane. The carbon atoms in the cyclohexane molecules are blue while the carbon atoms in the benzene molecule are green. Hydrogen atoms are omitted. Grey lines identify the location of a four-molecule plane in each structure.

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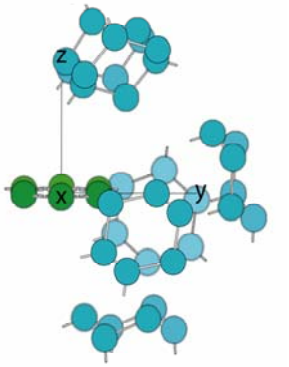
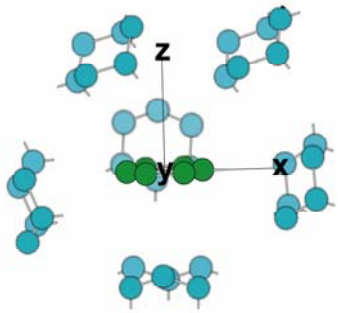
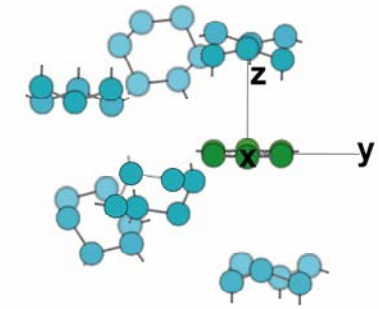
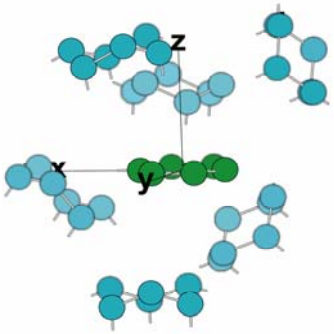
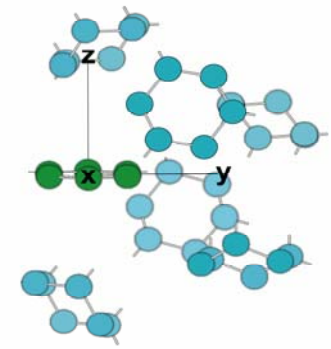
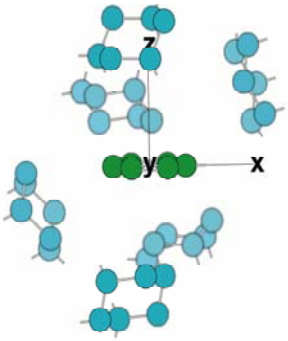
Group 1		
	Structure 27 **Side View x,y-plane**	**Structure 27** **Front View x,y-plane**
1A		
	Structure 21 **Side View x,y-plane**	**Structure 21** **Side View x,y-plane**
1B		
	Structure 25 **Side View x,y-plane**	**Structure 25** **Front View x,y-plane**
1C		

Figure S5. Representative structures for each BC_6 Group 1 subgroup. Structures are shown from two different views of the x, y-plane. The carbon atoms in the cyclohexane molecules are blue while the carbon atoms in the benzene molecule are green. The hydrogen atoms are omitted for clarity.

S II. Structural Grouping, Properties, and Energies of BC_n Cluster Groups: BC_6

S. II. A. BC_6 *Group 1.* Group 1 structures have three cyclohexanes above and three below the x, y-plane, forming an evenly distributed half shell, containing two cap molecules, that partially encases the benzene moiety (**Figure S5**). Molecular coordinates of structures in the three subgroups (1A, 1B, and 1C) are listed in **Tables S31-S33**.

For subgroup 1A, the average R^2 value from the linear plane fit is 0.494, indicating a moderate fit (**Table S69**). Structures in this subgroup have the smallest distance deviations relative to the model PBP (**Figure S5, Table S70**). Angle deviation calculations suggest that benzene occupies an axial position in the quasi-PBP structure.

The average R^2 value for subgroup 1B structures is 0.819, indicating a reasonably good 5-molecule fit to a plane (**Table S69**). Relative distance deviations, however, are large, suggesting significant distortion from the PBP (**Table S70**). Because benzene is a member of the five-molecule plane, it occupies an equatorial position.

The average R^2 value obtained from the linear plane fit for subgroup 1C structures is 0.229; a five-molecule plane is not present (**Table 8**). This, combined with large distance and angle deviations, suggests that subgroup 1C structures are quite distorted from the PBP. Of the 28 isomers of BC_6, 11 (~39 %) belong to Group 1. Among these, two (~7%) are in subgroup 1A, two (~7%) in 1B, and seven (~25%) in 1C.

S. II, B. BC_6 *Group 2.* Group 2 structures have two cyclohexanes on one side of the x, y-plane with the remaining four on the opposite side. Molecular coordinates for structures belonging to Group 2 (subgroups 2A & 2B) are tabulated in **Tables S34-S35**. Subgroup 2A isomers have cyclohexanes forming a near-evenly distributed half shell, restricted to one side of benzene's hexagon. The average R^2 value for these structures is 0.472, indicating a moderate fit to a five-molecule plane (**Table S69**).

The relatively small distance and angle deviations confirm that structures of subgroup 2A are quasi PBP structures with the benzene moiety occupying an axial position (**Figure S6, Table S70**).

Table S69. Average regression coefficients (R^2) from the 3-D linear regression to a 5-molecule plane for each BC_6 subgroup.

Subgroup	Average R^2
1A	0.49
1B	0.82
1C	0.23
2A	0.47
2B	0.36
3A	0.95
3B	0.42
4A	0.26
4B	1.00
4C	0.27

Table S70. The average benzene energy ratio (Ben. E. Ratio) and cluster energy ratio (Cluster E. Ratio) for each subgroup of BC_6 structures (with standard deviations) . The average CM-to-molecule and molecule-to-molecule distance deviations from the model PBP are tabulated, as are the average axial vs. equatorial angle deviations.

			Ave. % Distance Dev.		Ave. % Angle Dev.	
Subgroup	**Ave. Ben. E. Ratio % (*Std. Dev.*)**	**Ave. Cluster E. Ratio % *(Std. Dev.)***	**CM-to-molecule *(Std. Dev) (%)***	**Molecule-to-molecule *(Std. Dev.) (%)***	**Axial *(Std. Dev.)(%)***	**Equatorial *(Std. Dev.)(%)***
1A	91.4 (*1.2*)	100.0 (*0.0*)	8.6 (*2.3*)	9.4 (*1.2*)	9.0 (*0.0*)	54.9 (*4.1*)
1B	97.8 (*0.6*)	97.7 (*2.2*)	15.8 (*0.1*)	14.1 (*2.7*)	29.1 (*0.4*)	24.3 (*5.9*)
1C	94.1 (*10.1*)	98.6 (*0.8*)	13.4 (*1.5*)	15.7 (2.0)	27.0 (*3.4*)	24.0 (*5.9*)
2A	97.6 (--)	100 (--)	8.4 (--)	12.6 (--)	13.5 (--)	43.0 (--)
2B	80.8 (*2.9*)	95.1 (*1.1*)	17.7 (*4.9*)	22.5 (*4.7*)	28.7 (*5.8*)	25.8 (*9.7*)
3A	63.6 (--)	98.5 (--)	10.9 (--)	29.4 (--)	27.5 (--)	25.0 (--)
3B	67.9 (*10.2*)	96.1 (*2.5*)	15.3 (*4.0*)	21.0 (*3.0*)	23.6 (*1.6*)	23.4 (*9.5*)
4A	65.2 (--)	97.5 (--)	12.9 (--)	17.4 (--)	13.7 (--)	40.4 (--)
4B	64.8 (--)	98.3 (--)	10.4 (--)	23.2 (--)	25.4 (--)	10.8 (--)
4C	62.7 (*3.77*)	98.3 (*0.9*)	11.8 (*5.1*)	22.1 (*2.7*)	22.5 (*3.0*)	17.9 (*7.8*)

Structures in subgroup 2B have a 5-member cyclohexane shell, with the sixth cyclohexane exterior to the shell. A triangular cyclohexane ring is present, separating the benzene molecule from the exterior cyclohexane (**Figure S6**). The average R^2 value for subgroup 2B is 0.358, indicating absence of a five-molecule plane (**Table S69**). This, coupled with the relatively large distance and angle deviations, indicates that subgroup 2B structures do not resemble a PBP (**Table S70**). Of the 28 BC_6 structures, six (~21%) belong to Group 2: one (~4%) belongs to subgroup 2A while five (~18%) are in 2B.

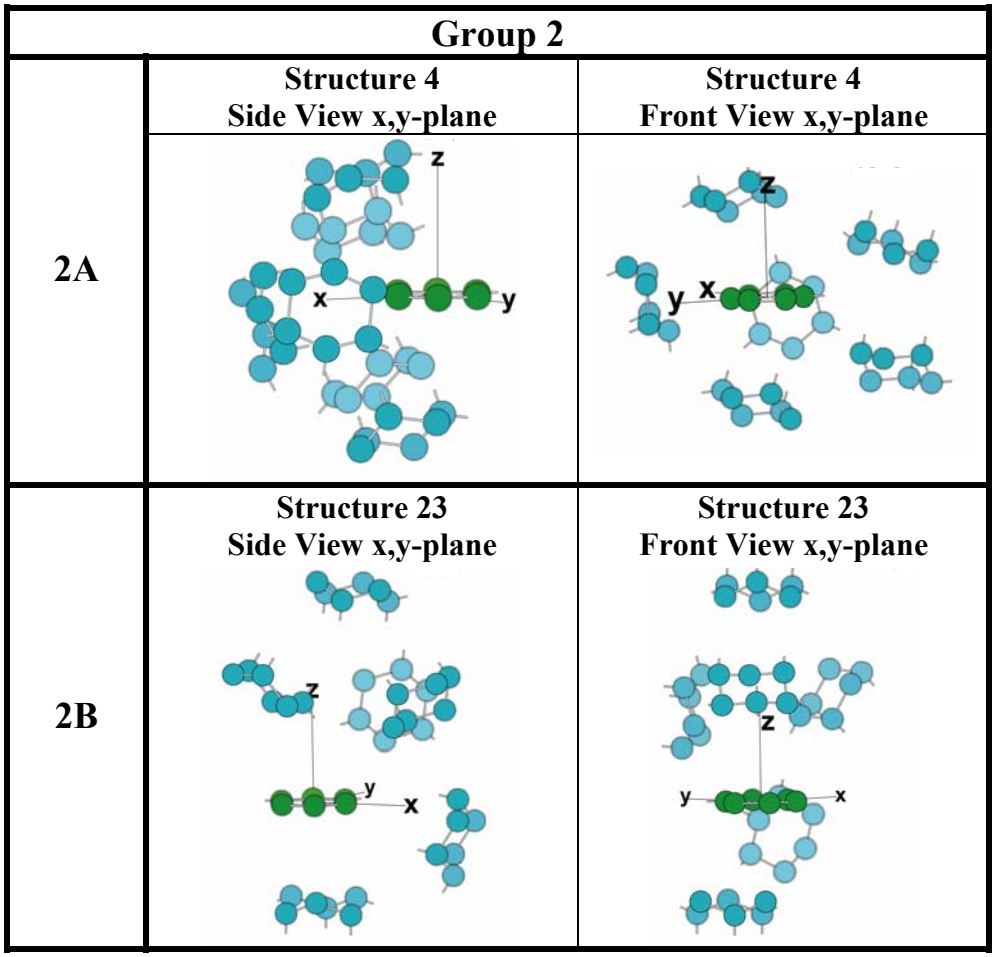


Figure S6. Representative structures of the BC_6 Group 2 subgroups. Structures are shown from two different views in the x, y-plane. The carbon atoms in the cyclohexane molecules are blue while the carbon atoms in the benzene molecule are green. Hydrogen atoms are not shown.

S. II. C. BC_6 *Group 3.* The structures of Group 3 have five cyclohexanes located on one side of the x, y-plane, with one on the opposite side. Molecular coordinates for subgroups 3A and 3B are collected in **Tables S36-S37**. Subgroup 3A structures are characterized by a cyclohexane half shell containing two nonparallel cap molecules (**Figure S7**). For the regression to a plane, the R^2 value is 0.949, confirming the presence of a five-molecule plane (**Table S69**). However, the distance and angle deviation calculations reveal significant distortion from a PBP. Because benzene is a member of the five-molecule plane, it occupies an equatorial position (**Table S70**).

The cyclohexane molecules in subgroup 3B structures encircle the z-axis (**Figure S7**). The 5-molecule plane fit yields an average R^2 of 0.421, indicating a moderate fit (**Table S69**). However, the distance and angle deviations are relatively large (**Table S70**), indicating significant departure from the PBP structure. Of the 28 BC_6 isomers, four (~14%) belong to Group 3. One (~4%) is in subgroup 3A and three (~11%) are in 3B.

III.E.1.d. BC_6 *Group 4.* In Group 4 structures, all six cyclohexane CMs are positioned on the same side of the x, y-plane (**Figure S8**). Molecular coordinates of structures representing the three Group 4 subgroups are provided in **Tables S38**-**S40**. Subgroup 4A structures have a five-member cyclohexane ring separating the benzene molecule from the sixth cyclohexane moiety; both non-ring molecules are horizontally oriented (**Figure S8**). The arrangement mimics the PBP structure with benzene occupying an axial position, as confirmed by relatively small distance and angle deviations (**Table S70**). However, the five-molecule ring is non-planar, indicated by the small R^2 value (0.260) (**Table S69**).

In subgroups 4B and 4C there is no 5-member cyclohexane ring. However, the R^2 value for subgroup 4B structures is 0.998, indicating the presence of a 5-molecule plane containing benzene (see **Figure S8**). The distance and angle deviations are relatively large, but angle analysis confirms that benzene occupies the equatorial position in a PBP structure (**Table S70** and **Figure S8**). For subgroup 4C, the R^2 value is 0.266 and both the distance and angle deviations are relatively large (**Tables S69** and **S70**), indicating substantial deviation from a PBP structure. Of the 28 simulated structures of BC_6, seven (~25%) belong to Group 4. One (~4%) belongs to subgroup 4A, one (~4%) belongs to subgroup 4B (~4%), and five (~18%) are in 4C.

S. II. D. Energy Comparisons for BC_6 Structural Groups

Table S70 presents the benzene- and total cluster energy stabilization ratios for each subgroup. Total cluster energy ratios range from 95 - 100% for all subgroups; however, a distinction is observed in the benzene-molecule stabilization. Subgroups 1A, 1B, 1C and 2A, all of which possess a six-member

cyclohexane half shell, have large benzene stabilization ratios (91-98%, **Table S70**). Subgroups 3A, 3B, 4A, 4B and 4C, in which the benzene molecule is more isolated, have much smaller benzene ratios (62-68%, **Table S70**). In the latter structures, a minimum of five cyclohexane molecules are positioned on the same side of the x, y-plane.

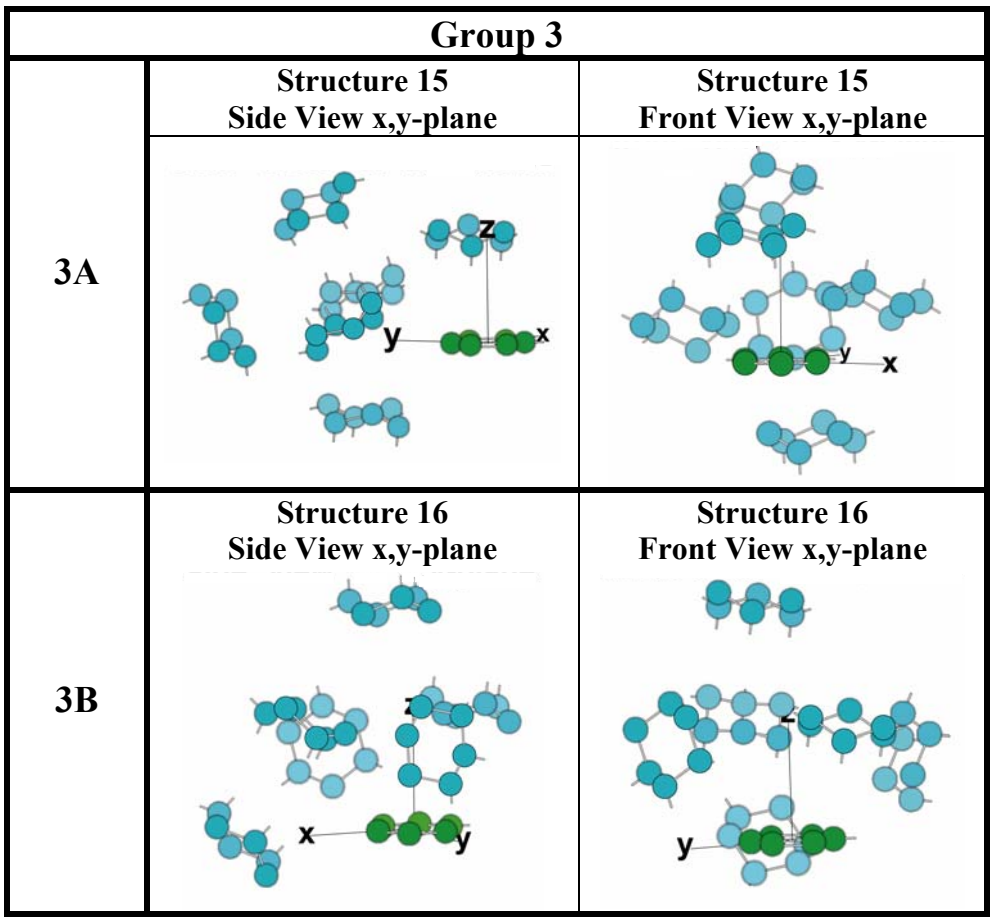


Figure S7. Representative structures for BC_6 Group 3 clusters, shown from two different perspectives in the x, y-plane. Carbon atoms in the cyclohexane molecules are blue; carbon atoms in benzene are green. Hydrogen atoms are not shown.

Group 4		
4A	Structure 13 Side View x,y-plane	Structure 13 Front View x,y-plane
4B	Structure 12 Side View x,y-plane	Structure 12 Side View x,y-plane
4C	Structure 1 Side View x,y-plane	Structure 1 Front View x,y-plane

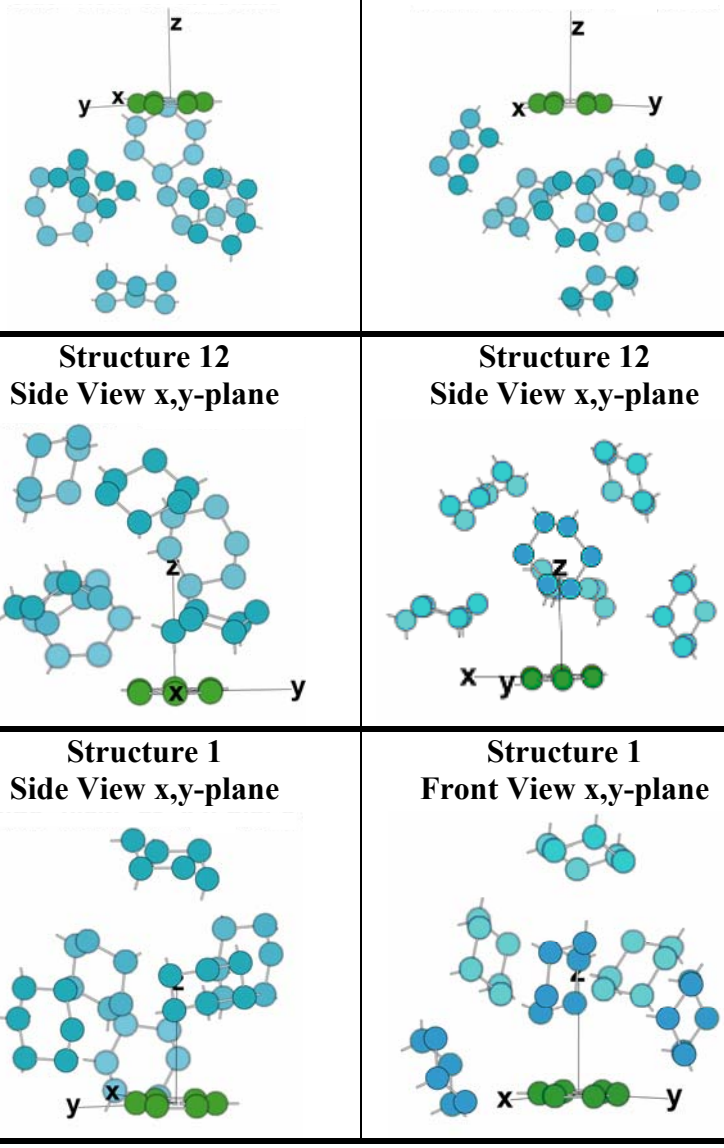


Figure S8. Representative structures of BC_6 Group 4 clusters, each presented from two different perspectives in the x, y-plane. Carbon atoms in the cyclohexane molecules are blue; carbon atoms in benzene are green. Hydrogen atoms are not shown.

S III. Structural Grouping, Properties, and Energies of BC_n Cluster Groups: BC_7

S. III. A. BC_7 *Group 1.* In Group 1, the cyclohexane moieties form an evenly distributed half shell containing two cap molecules; the shell partially encases the benzene molecule (**Figure S7**). The cyclohexanes are distributed either 5-2 or 4-3 with respect to the x, y-plane. In subgroup 1A, all seven cyclohexanes are restricted to the same half of the benzene hexagon. In subgroup 1B structures, one of the cap molecules is positioned on the opposite half of the benzene hexagon, relative the other six (**Figure S9**). In addition, a triangular cyclohexane ring, containing the aforementioned cap molecule, is present in subgroup 1B. Of the 14 BC_7 structures, 12 (~86%) belong to Group 1. Eleven of these (~79 %) are in subgroup 1A, and one (~7 %) is in subgroup 1B.

S. III. B. BC_7 *Group 2.* Molecular coordinates of Group 2 structures are tabulated in **Table S45**. These have six or seven cyclohexanes positioned on the same side of the x, y-plane. The cyclohexane molecules do not form a half shell around the benzene molecule; rather, they clump together in one quadrant (**Figure S9**). In addition, a three- or four-member cyclohexane ring structure is observed. Two (~14%) of the 14 BC_7 structures belong to Group 2.

S.III. C. Energies and Distance Deviations of BC_7 Structural Groups

The average benzene and cluster energy stabilization ratios for each subgroup of BC_7 clusters are shown in **Table S7**. Corresponding values for the individual BC_7 structures are collected in **Table S46**. The benzene molecular stabilization ratio is most favorable in Groups 1A and 1B, where a cyclohexane half-shell partially encases the benzene moiety. In Group 2, the cyclohexane molecules are clumped in one quadrant, with decreased benzene-cyclohexane interactions. Regarding total cluster energy, all subgroups range from 97 – 100%, with Group 2 energies being slightly more favorable than those of Group 1 (**Table S7**).

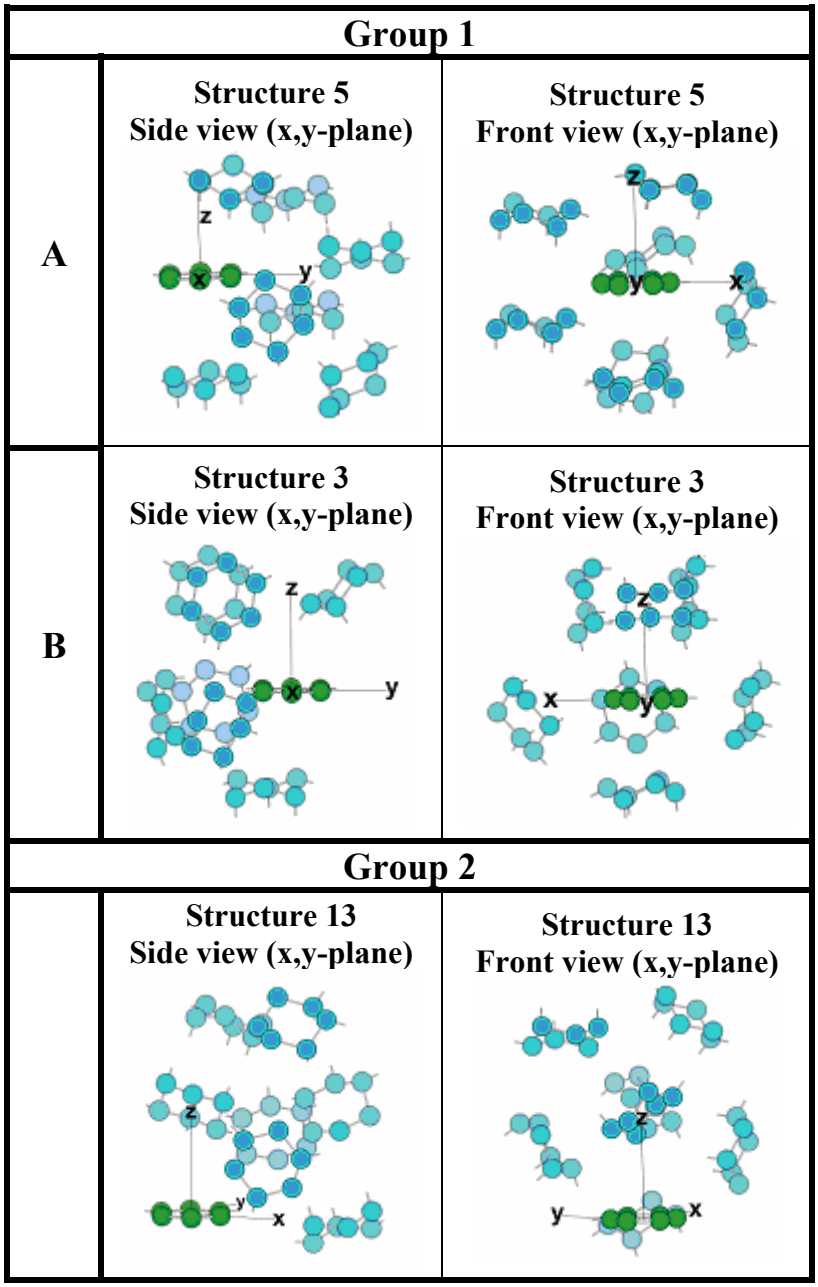


Figure S9. Representative structures of BC_7 clusters, shown from two different perspectives of the x, y-plane. The carbon atoms in the cyclohexane molecules are blue; carbon atoms in benzene are green. The hydrogen atoms are not shown.

Table S71. The average Benzene energy ratio (Ben. E.) and Cluster energy ratio (Cluster E.) for each subgroup of BC_7 clusters, along with their corresponding standard deviation (Std. Dev.). Also included are deviations from the cluster CM-to-molecule and molecule-to-molecule distances, relative to the model hexagonal bipyramid.

Properties	Subgroup 1A	Subgroup 1B	Group 2
Ave. Ben E. Ratio (%)	90.8	99.6	49.3
Std. Dev.	8.0	--	5.2
Ave. Cluster E. Ratio (%)	98.3	97.8	99.5
Std. Dev.	0.9	--	0.1
Ave. Distance Dev.			
CM-to-Molecule (%)	14	16	12
Std. Dev.	4	--	3
Molecule-to-molecule (%)	17	12	24
Std. Dev.	5	--	1

S IV. Structural Grouping, Properties, and Energies of BC_n Cluster Groups: BC_{12}

S. IV. A. BC_{12} *Group 1.* The molecular coordinates of Group 1 structures are listed in **Table S48**. The twelve cyclohexane molecules form a complete shell encasing the benzene moiety; this group most closely resembles the model icosahedron (**Figure S10**), a conclusion confirmed by the distance and angle deviation analysis (**Tables S54** and **S72**). Of the 20 BC_{12} structures, six (~30%) have the quasi-icosahedral structure of Group 1.

S. IV. B. BC_{12} *Group 2.* The molecular coordinates for Group 2 structures are listed in **Table S49**. These structures have an incomplete, 11-cyclohexane shell surrounding the interior benzene, with the twelfth C_6H_{12} molecule outside the shell (**Figure S10, Table S72**). Benzene occupies the central position within the incomplete shell (**Table S72**), as verified both by inspection of **Figure S73** and by distance and angle deviation analysis that excludes the twelfth cyclohexane molecule (**Table S73)**. Of the twenty BC_{12} structures, two (~10%) are in Group 2.

Table S72. The average Benzene energy (Ben. E.) and Cluster energy (Cluster E.) for each BC_{12} cluster group, along with the corresponding standard deviation (Std. Dev.) . Also included are average distance deviations for the cluster CM-to-molecule, benzene in the "inner" vs. "outer" positions, and angle deviations for "inner" vs. "outer" positions.

Properties	**Group 1**	**Group 2**	**Group 3**	**Group 4**	**Group 5**	**Group 6**
Ave. Ben E. (%)	99.6	90.8	89.5	78.8	72.7	66.4
Std. Dev.	0.7	1.0	--	5.8	2.0	--
Ave. Cluster E. (%)	99.9	95.6	96.5	95.0	92.9	99.6
Std. Dev.	0.3	1.1	--	0.7	1.2	--
Ave. Distance Dev.(%)						
CM-to-Molecule	4.8	14.2	16.4	19.5	22.2	22.9
Std. Dev.	1.1	1.6	--	1.6	1.6	--
Inner	5.7	15.7	18.3	23.3	24.0	29.9
Std. Dev.	1.6	1.0	--	2.0	1.7	--
Outer	23.4	17.6	17.6	16.4	13.9	12.0
Std. Dev.,	1.3	0.00	--	0.8	1.2	--
Ave. Angle Dev.(%)						
Inner	12.1	10.0	13.0	10.5	13.0	8.7
Std. Dev.	1.7	2.8	--	1.1	1.8	--
Outer	14.6	12.2	15.1	12.3	14.8	10.7
Std. Dev.	1.8	2.9	--	1.0	1.9	--

S. IV. C. BC_{12} *Groups 3-6*. The key difference between Groups 3-6 is in the number of cyclohexane molecules forming the partial shell structure around the benzene moiety. Specifically, the number of cyclohexanes in the partial shell decreases by one with each increase in group number: Group 3's partial solvation shell has 10 members, Group 4's has 9, Group 5's has 8, and Group 6's has 7. In all cases, the benzene moiety is partially surrounded by the majority of cyclohexane molecules (**Table S73**), with the remaining cyclohexanes positioned outside of the partial shell (**Figure S73**). Molecular coordinates of individual structures in Groups 3-6 are tabulated in **Tables S50 – S53**. Of the 20 BC_{12} structures, one is in Group 3, four are in Group 4, six are in Group 5, and one is in Group 6.

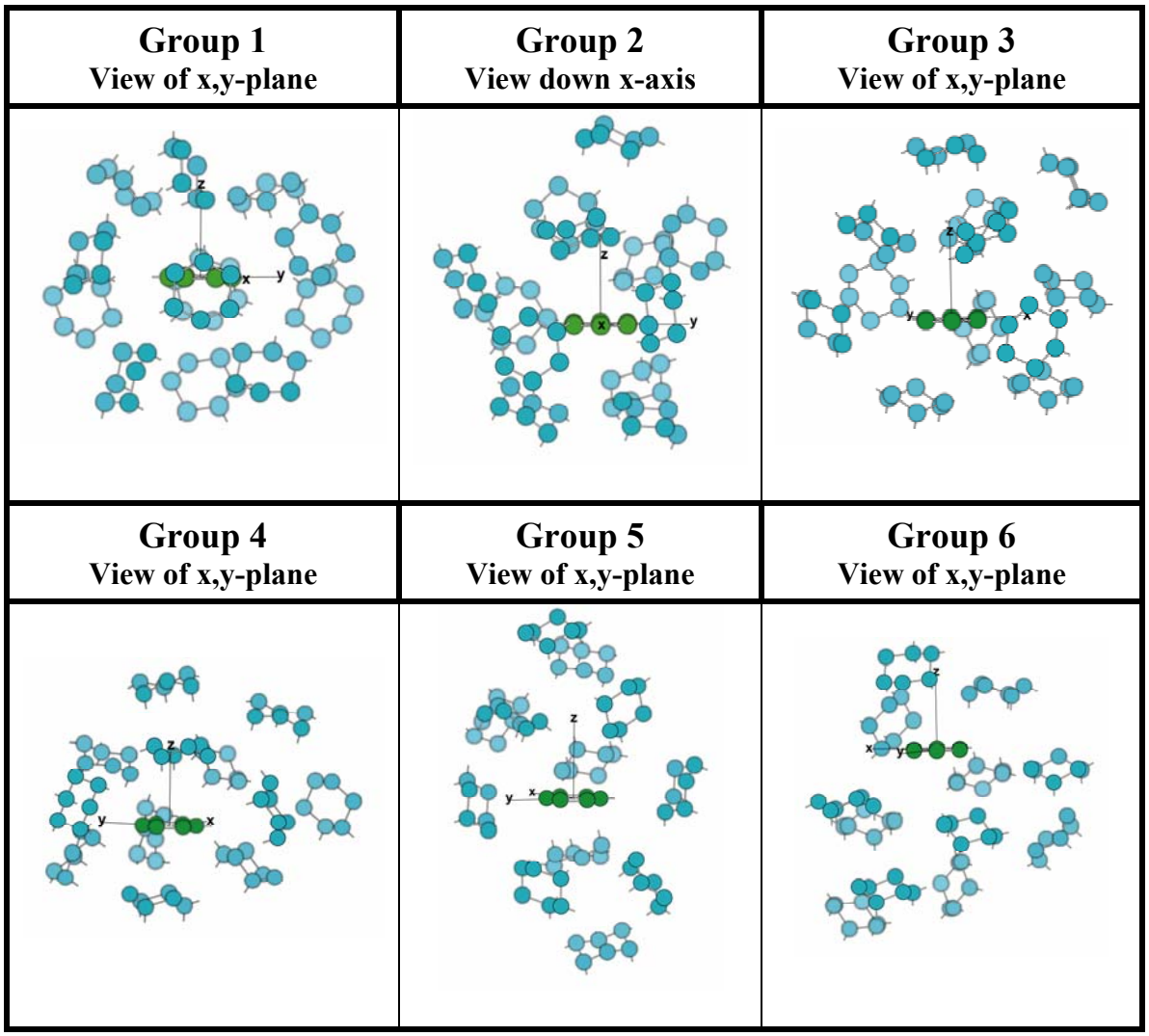


Figure S10. Representative structures of the six BC_{12} cluster groups, viewed from the x, y-plane. The carbon atoms in cyclohexane are blue; carbon atoms in benzene are green. Hydrogen atoms have been eliminated.

Table S73. Modified deviation calculations for BC_{12} Groups 2 – 6 that exclude the cyclohexanes moieties located exterior to the partial solvation shell. Cluster CM-to-molecule distance deviations and distance/ angle deviations for benzene in the "inner" vs. "outer" positions are shown.

Properties	Group 2	Group 3	Group 4	Group 5	Group 6
Ave. Distance Dev.(%)					
CM-to-Molecule	13.1	16.1	19.7	21.5	24.7
Std. Dev.	3.2	--	2.0	1.3	--
Inner	11.3	8.1	11.9	11.5	13.0
Std. Dev.	3.9	--	1.6	3.3	--
Outer	20.2	23.5	25.6	27.4	30.5
Std. Dev.,	0.5	--	1.2	1.8	--
Ave. Angle Dev.(%)					
Inner	9.9	12.0	10.2	13.7	6.8
Std. Dev.	2.9	--	2.6	1.6	--
Outer	12.1	13.6	12.0	15.5	8.0
Std. Dev.	3.0	--	2.3	1.6	--

Table S74. Characteristics of the BC_{12} clusters groups, including the number of cyclohexane molecules forming the full or partial shell, the cluster CM-to-molecule deviation, the benzene stabilization ratio, and the percentage simulation structures representing each group.

Group	Number of Cyclohexanes Forming Shell	CM-to-molecule % Deviation	Percentage of BC_{12} Clusters (%)	Ave. Ben E. Ratio (%)
1	12	4.8	30	99.6
2	11	14.2	10	90.8
3	10	16.4	5	89.5
4	9	19.5	20	78.8
5	8	22.2	30	72.7
6	7	22.9	5	66.4

S. IV. D. Energy Comparisons in BC_{12} Groups

Table S72 presents average distance and angle deviation results, along with benzene and cluster energy ratios. (Corresponding results for individual structures can be found in **Table S55**.) Total cluster energy ratios are between 95 - 100 % for all groups. The benzene-molecule stabilization decreases with increasing group number, as expected based on the number of benzene-cyclohexane nearest neighbors. Group 1, solvated by a complete shell, has the most favorable benzene stabilization, while Group 6, has the least (**Table S72**).