Supplementary Material (ESI) for PCCP

Stabilizing Carbon-Lithium Stars

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Cartesian coordinates and ZPE of C_5Li_n at B3LYP/def2-TZVPP level. The absolute energies (E) in hartrees and relative energies (ΔE) in kcal·mol^{-1} were calculated at CCSD(T)/def2-TZVPP//B3LYP/def2-TZVPP level.

Structure		Coordinates			E	ZPE	ΔE
1-A	6	-0.138849	-2.009772	0.000000	-227.4640662	0.029354	0.0
	6	1.102607	-1.806363	0.000000			
	3	-1.881972	-0.962057	0.000000			
	3	0.180105	-0.185215	1.214999			
	3	-2.900572	1.982437	0.000000			
	6	-1.267043	0.917505	0.000000			
	3	0.180105	-0.185215	-1.214999			
	3	2.446156	-0.270957	0.000000			
	6	1.291374	1.313305	0.000000			
	6	0.000000	1.395828	0.000000			
1-B	6	-0.464735	-2.046989	0.000000	-227.4597714	0.029568	2.8
	6	0.791385	-1.955674	0.000000			
	3	-2.085353	-0.792293	0.000000			
	3	0.044665	-0.257699	1.209447			
	3	-1.127815	2.945795	0.000000			
	6	-1.293514	1.021645	0.000000			
	3	0.044665	-0.257699	-1.209447			
	3	2.290677	-0.561725	0.000000			
	6	1.338779	1.145389	0.000000			
	6	0.044665	1.297440	0.000000			
1-C	6	0.000000	1.400345	0.000000	-227.4515362	0.028449	7.3
	6	1.330842	1.201382	0.000000			
	3	3.134560	1.059181	0.000000			
	3	-0.172434	0.075164	1.483843			
	6	-1.287931	1.277332	0.000000			
	3	-0.172434	0.075164	-1.483843			
	6	-0.537909	-1.836812	-0.626752			
	6	-0.537909	-1.836812	0.626752			
	3	-2.121666	-0.497194	0.000000			
	3	1.397787	-1.123183	0.000000			

1-D	3	-0.369181	0.122497	1.426818	-227.4448865	0.02964	12.2
	3	-1.717025	2.376156	-0.025737			
	6	-2.036827	0.482158	-0.190011			
	6	-1.424967	-0.629153	-0.137991			
	3	-0.011251	0.337805	-1.281314			
	6	-0.402536	-1.546104	0.025230			
	6	1.691410	-0.012367	0.235973			
	3	3.319194	0.470341	-0.736021			
	6	0.796265	-0.936016	0.124132			
	3	1.531572	1.976163	0.501586			
1-E	3	-2.750400	-0.014929	1.113289	-227.4434312	0.028658	12.5
	6	-0.895912	0.044346	-0.514965			
	6	1.916482	-1.117781	0.317572			
	6	-1.789717	-0.843805	-0.410080			
	6	1.314384	-0.124016	-0.171613			
	3	1.740457	1.971228	-0.060116			
	3	0.066450	-1.898157	-0.238905			
	6	0.279880	0.829835	-0.476183			
	3	0.266880	0.130264	1.567006			
	3	-0.973622	2.234438	0.129263			
1-F	3	0.499607	-0.118305	1.354827	-227.4419288	0.028765	13.5
	6	-0.543771	1.064482	0.000000			
	6	0.499607	1.794510	0.000000			
	3	2.461647	1.593649	0.000000			
	3	0.499607	-0.118305	-1.354827			
	3	2.392022	-1.785441	0.000000			
	3	-2.640510	1.305533	0.000000			
	6	-1.401606	-0.084444	0.000000			
	6	0.433339	-1.974872	0.000000			
	6	-0.593755	-1.238242	0.000000			
1-G	3	-0.335952	-1.539486	-0.410888	-227.4416601	0.028967	13.8
	3	1.639925	2.097473	0.455578			
	3	-0.770111	0.747881	1.421245			
	3	-3.257599	-0.775061	0.940163			
	6	1.800088	-1.240443	-0.250512			
	6	0.359635	1.009006	-0.478586			
	6	1.224259	-0.125158	-0.392938			
	6	-2.009518	-0.099715	-0.335521			
	6	-0.935983	0.532771	-0.573489			
	3	1.846777	-0.683729	1.655994			

1-H	3	0.000000	1.912475	-1.881137	-227.4413636	0.02935	14.2
	3	1.322785	0.000000	0.025952			
	6	0.000000	0.000000	1.834230			
	3	-1.322785	0.000000	0.025952			
	6	0.000000	1.128827	1.059493			
	6	0.000000	-1.128827	1.059493			
	6	0.000000	-1.874032	0.022264			
	6	0.000000	1.874032	0.022264			
	3	0.000000	0.000000	-4.285120			
	3	0.000000	-1.912475	-1.881137			
1-I	6	2.841020	0.052308	-0.307115	-227.4409302	0.029431	14.6
	6	1.595090	0.001093	-0.492669			
	6	0.272697	-0.048950	0.000989			
	3	1.800313	-1.357935	0.866753			
	3	1.534477	1.374477	0.924933			
	6	-0.979399	-0.246949	-0.560007			
	6	-2.247683	-0.225510	-0.555602			
	3	-1.077504	-0.665222	1.446286			
	3	-1.323056	1.562939	0.234282			
	3	-3.897683	0.021755	0.356555			
1-J	6	0.000000	0.824506	-1.089271	-227.4104617	0.031372	34.9
	6	0.000000	-0.824506	-1.089271			
	6	0.000000	-1.246822	0.244419			
	6	0.000000	0.000000	1.105172			
	6	0.000000	1.246822	0.244419			
	3	-1.633821	0.000000	-0.140834			
	3	1.633821	0.000000	-0.140834			
	3	0.000000	0.000000	-2.767473			
	3	0.000000	-1.601100	2.109102			
	3	0.000000	1.601100	2.109102			
1-K	6	0.000000	1.231505	0.000000	-227.3954315	0.031608	44.5
	6	1.171230	0.380556	0.000000			
	6	0.723860	-0.996308	0.000000			
	6	-0.723860	-0.996308	0.000000			
	6	-1.171230	0.380556	0.000000			
	3	1.600306	2.202633	0.000000			
	3	2.589350	-0.841331	0.000000			
	3	0.000000	-2.722604	0.000000			
	3	-2.589350	-0.841331	0.000000			
	3	-1.600306	2.202633	0.000000			

2-A	3	0.444689	0.001135	1.238137	-234.9457844	0.031441	0.0
	6	2.252045	0.184295	-0.000258			
	6	1.923382	-1.026258	-0.000322			
	3	0.444204	0.001611	-1.237926			
	6	-0.541149	1.551664	0.000862			
	3	1.417634	2.030942	0.000504			
	6	-1.313612	-0.957719	-0.000166			
	6	-1.097458	0.355412	0.000450			
	3	-2.343970	2.143689	-0.001961			
	3	0.327316	-2.223793	-0.000612			
	3	-2.736288	-2.168369	0.000727			
2-B	3	1.498134	0.000000	-0.147432	-234.9412655	0.031007	2.6
	6	0.625952	0.000000	-2.047366			
	6	-0.625952	0.000000	-2.047366			
	3	0.000000	1.763503	-1.020571			
	6	0.000000	1.306879	1.002481			
	3	0.000000	2.834855	2.077948			
	6	0.000000	0.000000	1.179824			
	3	-1.498134	0.000000	-0.147432			
	6	0.000000	-1.306879	1.002481			
	3	0.000000	-2.834855	2.077948			
	3	0.000000	-1.763503	-1.020571			
2-C	6	1.346488	0.883987	0.000000	-234.9407824	0.030589	2.6
	3	0.525409	2.852938	0.000000			
	3	-0.287658	-0.168396	1.594346			
	3	1.317110	-1.246742	0.000000			
	3	3.158263	1.112059	0.000000			
	6	0.000000	1.036909	0.000000			
	6	-0.589955	-1.976386	0.625545			
	6	-0.589955	-1.976386	-0.625545			
	6	-1.279977	1.161040	0.000000			
	3	-2.198667	-0.639791	0.000000			
	3	-0.287658	-0.168396	-1.594346			
2-D	3	0.000000	0.000000	1.586033	-234.9411696	0.035935	5.7
	3	1.615874	2.224060	-0.163045			
	3	2.614540	-0.849515	-0.163045			
	6	0.000000	1.240667	-0.077081			
	6	1.179944	0.383387	-0.077081			
	6	0.729246	-1.003720	-0.077081			
	6	-1.179944	0.383387	-0.077081			
	3	-2.614540	-0.849515	-0.163045			
	6	-0.729246	-1.003720	-0.077081			
	3	0.000000	-2.749090	-0.163045			
	3	-1.615874	2.224060	-0.163045			

2-E	6	0.824875	-1.628849	0.000000	-234.9331739	0.031944	8.2
	6	-0.442163	-1.746370	0.000000			
	3	-2.187390	-0.571027	0.000000			
	3	0.037667	0.015058	1.254558			
	3	-1.370579	3.081576	0.000000			
	3	0.362833	-3.566818	0.000000			
	6	0.000000	1.498317	0.000000			
	6	1.293338	1.343332	0.000000			
	6	-1.312965	1.161307	0.000000			
	3	2.393633	-0.229322	0.000000			
	3	0.037667	0.015058	-1.254558			
2-F	6	0.000000	0.722604	-1.189935	-234.933282	0.0355	10.4
	6	0.000000	1.181328	0.233740			
	3	0.000000	1.642392	2.083532			
	3	-1.657328	0.000000	-0.211114			
	3	1.657328	0.000000	-0.211114			
	6	0.000000	-1.181328	0.233740			
	6	0.000000	0.000000	1.110355			
	6	0.000000	-0.722604	-1.189935			
	3	0.000000	-2.597385	-1.070383			
	3	0.000000	2.597385	-1.070383			
	3	0.000000	-1.642392	2.083532			
3-A	6	0.000000	1.249288	0.000000	-242.3423067	0.038412	0.0
	3	2.663026	-0.865270	0.000000			
	3	1.645841	2.265306	0.000000			
	3	-1.645841	2.265306	0.000000			
	3	0.000000	0.000000	1.687897			
	3	0.000000	0.000000	-1.687897			
	6	-0.734313	-1.010695	0.000000			
	6	-1.188143	0.386051	0.000000			
	3	0.000000	-2.800072	0.000000			
	3	-2.663026	-0.865270	0.000000			
	6	0.734313	-1.010695	0.000000			
	6	1.188143	0.386051	0.000000			

3-B	6	0.000000	0.000000	1.380238	-242.3206823	0.033457	10.5
	3	0.000000	2.497460	2.640366			
	3	1.281877	0.000000	-0.115057			
	3	0.000000	2.266511	-0.591760			
	3	-1.281877	0.000000	-0.115057			
	6	0.000000	1.300457	1.152536			
	6	0.000000	0.630350	-1.859244			
	6	0.000000	-0.630350	-1.859244			
	3	0.000000	-2.266511	-0.591760			
	3	0.000000	0.000000	-3.800742			
	3	0.000000	-2.497460	2.640366			
	6	0.000000	-1.300457	1.152536			
3-C	6	0.000000	1.262854	0.000000	-242.2204972	0.032727	72.9
	6	1.201045	0.390243	0.000000			
	6	0.742287	-1.021670	0.000000			
	6	-0.742287	-1.021670	0.000000			
	6	-1.201045	0.390243	0.000000			
	3	0.000000	3.217360	0.000000			
	3	3.059892	0.994219	0.000000			
	3	1.891117	-2.602899	0.000000			
	3	-1.891117	-2.602899	0.000000			
	3	-3.059892	0.994219	0.000000			
	3	0.000000	0.000000	1.648599			
	3	0.000000	0.000000	-1.648599			
Most stable triplet	6	0.134864	-2.652739	0.000000	-242.2708881	0.030188	39.7
	6	0.953023	-1.713907	0.000000			
	6	-0.274925	1.192784	1.305866			
	6	-0.274925	1.192784	-1.305866			
	6	-0.353478	1.101888	0.000000			
	3	-0.321740	-4.535243	0.000000			
	3	1.591426	0.220940	0.000000			
	3	-0.482323	3.077719	0.000000			
	3	-0.303314	-0.899734	1.491883			
	3	-0.274925	2.397217	2.843836			
	3	-0.274925	2.397217	-2.843836			
	3	-0.303314	-0.899734	-1.491883			