Supporting Information available for

Smallest deltahedra silicon dicarbide: $C_2Si_3^{2-}$

Jing-jing Sui, Jing Xu, Yi-hong Ding*

Institute of Theoretical Chemistry, Jilin University, Changchun 130023, People's Republic of China.

S1. Table S1. For all the singlet $C_2Si_3^{2-}$ isomers , the energies(in a.u.), zero-point energies(in a.u.), the relative energies(in kcal/mol) at B3LYP/aug-cc-pVTZ,CCSD(T)/ aug-cc-pVTZ//B3LYP/aug-cc-pVTZ and PBE0/cc-pVTZ//B3LYP/aug-cc-pVTZ.

S2.Table S2. For all the triplet $C_2Si_3^{2-}$ isomers, the energies(in a.u.), zero-point energies(in a.u.), the relative energies(in kcal/mol) at B3LYP/aug-cc-pVTZ and CCSD(T)/ aug-cc-pVTZ //B3LYP/aug-cc-pVTZ.

S3. Table S3. For the $CpMg(C_2Si_3^{2-})MgCp$, the energies(in a.u.), zero-point energies(in a.u.), the relative energies(in kcal/mol) at B3LYP/6-31g(d) and PBE0/ cc-pVTZ //B3LYP/6-31g(d).

S4. Table S4. Cartesian coordinates of the isomers in Table S1 at the level of B3LYP/aug-cc-pVTZ.

S5. Table S5. Cartesian coordinates of the isomers in Table S2 at the level of B3LYP/aug-cc-pVTZ.

S6. Table S6. Cartesian coordinates of the isomers in Table S3 at the level of B3LYP/6-31g(d).

S1. Table S1. For all the singlet isomers, the energies(in a.u.), zero-point energies(in a.u.), the relative energies(in kcal/mol) at B3LYP/aug-cc-pVTZ, CCSD(T)/ aug-cc-pVTZ //B3LYP/aug-cc-pVTZ and PBE0/ cc-pVTZ //B3LYP/aug-cc-pVTZ

	B3LYP/ aug-cc-pVTZ			CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ			PBE0 /cc-pVTZ//B3LYP/ aug-cc-pVTZ		
	E	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE
C2Si32-_020	-944.617433	-944.607153	11.1	-943.082691	-943.072411	0	-944.108196	-944.097916	0
C2Si32-_019	-944.631112	-944.620571	2.68	-943.082781	-943.07224	0.10730421	-944.105182	-944.094641	2.0550953
C2Si32-_015	-944.635952	-944.624848	0	-943.081105	-943.070001	1.5122991	-944.103143	-944.092039	3.6878763
C2Si32-_009	-944.613658	-944.602808	13.83	-943.069278	-943.058428	8.77447233	-944.084504	-944.073654	15.224648
C2Si32-_001	-944.609815	-944.600025	15.57	-943.063958	-943.054168	11.44766493	-944.08225	-944.07246	15.973895
C2Si32-_023	-944.588033	-944.578056	29.36	-943.059779	-943.049802	14.18737359	-944.081196	-944.071219	16.752634
C2Si32-_002	-944.604119	-944.594193	19.23	-943.054508	-943.044582	17.46297579	-944.063698	-944.053772	27.700801
C2Si32-_011	-944.604299	-944.594709	18.91	-943.051307	-943.041717	19.26079194	-944.066932	-944.057342	25.460591
C2Si32-_073	-944.602655	-944.592264	20.44	-943.042447	-943.032056	25.32316605	-944.061174	-944.050783	29.576429
C2Si32-_022	-944.559864	-944.550134	46.88	-943.031934	-943.022204	31.50539457	-944.045196	-944.035466	39.188
C2Si32-_041	-944.57554	-944.567098	36.23	-943.027319	-943.018877	33.59312034	-944.043092	-944.03465	39.700048
C2Si32-_010	-944.576029	-944.566218	36.79	-943.028208	-943.018397	33.89432514	-944.04531	-944.035499	39.167292
C2Si32-_012	-944.568949	-944.559341	41.1	-943.022165	-943.012557	37.55898354	-944.033786	-944.024178	46.271332
C2Si32-_005	-944.566458	-944.557271	42.4	-943.019379	-943.010192	39.04304469	-944.029062	-944.019875	48.971508
C2Si32-_038	-944.544165	-944.534784	56.51	-943.002291	-942.99291	49.88767251	-944.015164	-944.005783	57.814379
C2Si32-_016	-944.532687	-944.523804	63.4	-942.991582	-942.982699	56.29517712	-943.999386	-943.990503	67.402732
C2Si32-_018	-944.525887	-944.517554	67.32	-942.979649	-942.971316	63.43812345	-943.983431	-943.975098	77.069523
C2Si32-_004	-944.503204	-944.495291	81.29	-942.964566	-942.956653	72.63930258	-943.969255	-943.961342	85.701551
C2Si32-_070	-944.475781	-944.467512	98.72	-942.927781	-942.919512	95.94565149	-943.93531	-943.927041	107.22577
C2Si32-_072	-944.440913	-944.433938	119.79	-942.901719	-942.894744	111.4878192	-943.89957	-943.892595	128.84098

S2. Table S2. For all the triplet isomers, the energies(in a.u.), zero-point energies(in a.u.), the relative energies(in kcal/mol) at B3LYP/aug-cc-pVTZ and CCSD(T)/ aug-cc-pVTZ //B3LYP/aug-cc-pVTZ

	B3LYP/ aug-cc-pVTZ			CCSD(T)/aug-cc-pVTZ//B3LYP/aug-cc-pVTZ		
	E	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE
C2Si32-_073-tri	-944.621255	-944.610871	0	-943.058826	-943.048442	15.04078719
C2Si32-_005-tri	-944.617223	-944.607044	2.4	-943.056466	-943.046287	16.39307124
C2Si32-_136-tri	-944.59481	-944.584244	16.7	-943.052464	-943.041898	19.14721263
C2Si32-_108-tri	-944.608098	-944.596638	8.93	-943.052045	-943.040585	19.97113326
C2Si32-_034-tri	-944.596669	-944.587025	14.96	-943.045058	-943.035414	23.21598747
C2Si32-_001-tri	-944.589423	-944.579296	19.81	-943.042414	-943.032287	25.17821124
C2Si32-_025-tri	-944.587054	-944.577167	21.14	-943.041688	-943.031801	25.4831811
C2Si32-_020-tri	-944.588892	-944.578691	20.19	-943.039	-943.028799	27.36696612
C2Si32-_013-tri	-944.585294	-944.57548	22.2	-943.03648	-943.026666	28.70544495
C2Si32-_023-tri	-944.571923	-944.562704	30.22	-943.035729	-943.02651	28.80333651
C2Si32-_110-tri	-944.586885	-944.577055	21.21	-943.035533	-943.025703	29.30973708
C2Si32-_006-tri	-944.586551	-944.576825	21.36	-943.034525	-943.024799	29.87700612
C2Si32-_010-tri	-944.583893	-944.574285	22.95	-943.032456	-943.022848	31.10127813
C2Si32-_019-tri	-944.583902	-944.574027	23.11	-943.030419	-943.020544	32.54706117
C2Si32-_041-tri	-944.585526	-944.576079	21.83	-943.026425	-943.016978	34.78476183
C2Si32-_069-tri	-944.578732	-944.569569	25.91	-943.024873	-943.01571	35.58044451
C2Si32-_024-tri	-944.561462	-944.551926	36.98	-943.022709	-943.013173	37.17243738
C2Si32-_003-tri	-944.583205	-944.573638	23.36	-943.021339	-943.011772	38.05157889
C2Si32-_029-tri	-944.56665	-944.557157	33.7	-943.0136	-943.004107	42.86144304
C2Si32-_064-tri	-944.555669	-944.545899	40.77	-943.00509	-942.99532	48.37537341
C2Si32-_079-tri	-944.558097	-944.548639	39.05	-942.989395	-942.979937	58.02835974

C2Si32-_038-tri	-944.551341	-944.542478	42.91	-942.967078	-942.958215	71.65913196
C2Si32-_031-tri	-944.553483	-944.544059	41.92	-942.96721	-942.957786	71.92833375
C2Si32-_016-tri	-944.508169	-944.499818	69.68	-942.962158	-942.953807	74.42519604
C2Si32-_081-tri	-944.501474	-944.492506	74.27	-942.960233	-942.951265	76.02032646
C2Si32-_036-tri	-944.511451	-944.503152	67.59	-942.959109	-942.95081	76.30584351
C2Si32-_071-tri	-944.507796	-944.499733	69.74	-942.954894	-942.946831	78.8027058
C2Si32-_004-tri	-944.511027	-944.502964	67.71	-942.951638	-942.943575	80.84587836
C2Si32-_053-tri	-944.485356	-944.476819	84.11	-942.951808	-942.943271	81.0366414
C2Si32-_021-tri	-944.484193	-944.47592	84.68	-942.93937	-942.931097	88.67594814
C2Si32-_042-tri	-944.497629	-944.489779	75.98	-942.93746	-942.92961	89.60905551
C2Si32-_014-tri	-944.561469	-944.551446	37.28	-942.938134	-942.928111	90.549693
C2Si32-_072-tri	-944.439748	-944.432902	111.67	-942.888758	-942.881912	119.5400275
C2Si32-_105-tri	-944.435439	-944.428726	114.29	-942.878911	-942.872198	125.6356596
C2Si32-_134-tri	-944.410033	-944.403609	130.05	-942.859353	-942.852929	137.7271498
C2Si32-_011-tri	-944.395889	-944.388911	139.28	-942.824416	-942.817438	159.9981072

S3. Table S3. For the CpMg($C_2Si_3^{2-}$)MgCp, the energies(in a.u.), zero-point energies(in a.u.), the relative energies(in kcal/mol) at B3LYP/6-31g(d) and PBE0/ cc-pVTZ //B3LYP/6-31g(d).

	B3LYP/6-31g(d)			PBE0/ cc-pVTZ //B3LYP/6-31g(d).		
	E	E+ZPVE	ΔE+ZPVE	E	E+ZPVE	ΔE+ZPVE
C2Si3-CpMg-cage-1	-1731.90879	-1731.727784	0	-1730.998425	-1730.817419	0
CpMg-020-d2-t4	-1731.905887	-1731.725001	1.74	-1730.995271	-1730.814385	1.90386534
CpMg-023-d2-t2	-1731.889976	-1731.709931	11.2	-1730.985939	-1730.805894	7.23205275
CpMg-023-d1-t1	-1731.885242	-1731.705419	14.03	-1730.979942	-1730.800119	10.855923
CpMg-020-d2-t3	-1731.882836	-1731.702066	16.13	-1730.972953	-1730.792183	15.83584236
CpMg-015-d1-d2	-1731.89576	-1731.714966	8.04	-1730.971686	-1730.790892	16.64595777
C2Si3-CpMg-planar-1	-1731.895712	-1731.714912	8.07	-1730.971595	-1730.790795	16.70682624
C2Si3-CpMg-1-ptSi	-1731.880823	-1731.700342	17.22	-1730.970068	-1730.789587	17.46485832
C2Si3-CpMg-planar-C-C	-1731.887095	-1731.706369	13.43	-1730.963997	-1730.783271	21.42821148
CpMg-001-t1-s4	-1731.886925	-1731.706417	13.4	-1730.962306	-1730.781798	22.35253371
CpMg-009-d1-t3	-1731.874375	-1731.693589	21.45	-1730.961573	-1730.780787	22.98694632
CpMg-009-d1-d3	-1731.875683	-1731.694725	20.74	-1730.961385	-1730.780427	23.21284992
CpMg-001-d1-t2	-1731.886328	-1731.705404	14.04	-1730.961181	-1730.780257	23.31952662
CpMg-020-d4-t3	-1731.866326	-1731.686222	26.08	-1730.96019	-1730.780086	23.42683083
CpMg-026-s1-t1	-1731.874091	-1731.69375	21.35	-1730.959262	-1730.778921	24.15787998
CpMg-015-d1-s1	-1731.889576	-1731.708618	12.02	-1730.958739	-1730.777781	24.87324138
CpMg-001-d1-t5	-1731.884278	-1731.703284	15.37	-1730.957563	-1730.776569	25.6337835
CpMg-002-s1-t3	-1731.884243	-1731.704254	14.76	-1730.951007	-1730.771018	29.11709151
CpMg-001-d2-t2	-1731.868076	-1731.687898	25.02	-1730.951057	-1730.770879	29.2043154
CpMg-002-s1-t1	-1731.881095	-1731.70093	16.85	-1730.946687	-1730.766522	31.93837647
CpMg-015-d1-t1	-1731.875783	-1731.694873	20.65	-1730.94319	-1730.76228	34.60027389

CpMg-015-d1-s6	-1731.870561	-1731.690186	23.59	-1730.941856	-1730.761481	35.10165438
CpMg-011-s1-d8	-1731.844216	-1731.664695	39.58	-1730.91746	-1730.737939	49.8744948
CpMg-073-s1-t2	-1731.844916	-1731.664672	39.6	-1730.907164	-1730.72692	56.78902749

S4. Table S4. Optimized geometries (in angstrom) of the isomers in Table S1 at the level of B3LYP/aug-cc-pVTZ

C2Si32-_015.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.635952117 HF+ZPE=-944.624848 lf=117.0608
14 1.144748 1.652779 0.000000
6 0.000000 0.166427 0.000000
14 -1.140771 1.655842 0.000000
6 -0.001793 -1.173767 0.000000
14 -0.003209 -2.876904 0.000000

C2Si32-_019.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.631111917 HF+ZPE=-944.620571 lf=113.9393
14 1.203074 -1.453538 0.000000
14 0.000000 0.449575 0.000000
14 -1.202339 -1.454021 0.000000
6 -0.000645 2.241845 0.000000
6 -0.001070 3.493450 0.000000

C2Si32-_020.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.617432827 HF+ZPE=-944.607153 lf=216.2447
6 -1.563627 0.648006 0.000000
6 -0.322904 1.097437 0.000000
14 -0.322904 -0.680883 1.196295
14 1.454322 0.613719 0.000000
14 -0.322904 -0.680883 -1.196295

C2Si32-_009.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.613658042 HF+ZPE=-944.602808 lf=93.6546
14 -2.171298 -0.053734 0.000000
14 0.000000 0.997778 0.000000
6 -0.643497 -1.038700 0.000000
14 2.171299 -0.053729 0.000000
6 0.643496 -1.038699 0.000000

C2Si32-_001.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.609815423 HF+ZPE=-944.600025 lf=121.0979
6 -2.582439 -0.000037 0.646219
6 -1.462518 0.000053 0.055818
14 -0.014993 -1.289319 -0.360084
14 -0.014972 1.289331 -0.360068
14 1.763518 -0.000019 0.419279

C2Si32-_011.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.604298691 HF+ZPE=-944.594709 lf=46.6952

6 1.538434 -3.434673 0.000000
14 -0.701650 -1.380910 0.000000
6 0.737290 -2.465718 0.000000
14 0.000000 0.892706 0.000000
14 -0.273661 3.016943 0.000000

C2Si32-_002.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.604119328 HF+ZPE=-944.594193 lf=69.9889
6 -1.516340 0.061619 0.000000
14 -3.077500 -0.559242 0.000000
6 1.516300 0.061539 0.000000
14 3.077517 -0.559119 0.000000
14 0.000000 1.065579 0.000000

C2Si32-_073.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.602655273 HF+ZPE=-944.592264 lf=67.1370
14 0.019459 3.574464 0.000000
6 0.008661 1.804331 0.000000
6 0.000000 0.535491 0.000000
14 -0.006244 -1.218406 0.000000
14 -0.016927 -3.358839 0.000000

C2Si32-_023.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.588033305 HF+ZPE=-944.578056 lf=192.4568
14 0.517883 0.066070 1.604564
6 0.277284 0.994315 0.000000
6 0.517883 -0.892796 0.000000
14 0.517883 0.066070 -1.604564
14 -1.376552 -0.175648 0.000000

C2Si32-_010.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.576028560 HF+ZPE=-944.566218 lf=68.0082
6 1.584717 -1.724160 0.000000
6 0.502706 -0.892140 0.000000
14 -0.103870 -2.630651 0.000000
14 0.000000 0.891092 0.000000
14 -0.790739 2.860831 0.000000

C2Si32-_041.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.575539978 HF+ZPE=-944.567098 lf=46.6088
6 0.678652 -3.008545 0.000000
6 1.507940 -2.030865 0.000000
14 -0.558683 -1.530372 0.000000
14 0.000000 0.789061 0.000000

14 -0.378428 2.901059 0.000000

C2Si32-_012.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.568949473 HF+ZPE=-944.559341 lf=76.5461
6 1.517735 1.377795 0.000000
14 0.000000 0.374238 0.000000
14 0.201204 2.630682 0.000000
6 -0.303568 -1.379399 0.000000
14 -0.721561 -3.004232 0.000000

C2Si32-_005.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.566458356 HF+ZPE=-944.557271 lf=66.3182
14 1.772853 -0.822026 0.000000
6 0.000897 -1.157763 0.000000
6 0.000000 0.293422 0.000000
14 -1.771501 -0.824349 0.000000
14 -0.001736 2.016807 0.000000

C2Si32-_022.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.559863714 HF+ZPE=-944.550134 lf=315.7004
6 0.000000 1.373432 0.000024
14 0.000000 0.000000 1.389438
14 -1.202983 0.000000 -0.694729
6 0.000000 -1.373432 0.000024
14 1.202983 0.000000 -0.694729

C2Si32-_038.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.544165316 HF+ZPE=-944.534784 lf=91.8762
6 0.000000 1.723733 1.046935
14 0.000000 2.029535 -0.708454
14 0.000000 0.000000 0.519535
14 0.000000 -2.029535 -0.708454
6 0.000000 -1.723733 1.046935

C2Si32-_016.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.532686828 HF+ZPE=-944.523804 lf=17.0393
14 -1.169798 1.546137 0.000000
6 0.000000 0.132231 0.000000
14 1.157313 1.556284 0.000000
14 0.006979 -1.698942 0.000000
6 0.012846 -3.407013 0.000000

C2Si32-_018.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.525887227 HF+ZPE=-944.517554 lf=30.4907

14 -2.982082 -0.700331 0.000000
14 0.000000 1.044150 0.000000
6 -1.443498 -0.016159 0.000000
14 2.007380 -0.298151 0.000000
6 3.717801 -0.090400 0.000000

C2Si32-_004.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.503204081 HF+ZPE=-944.495291 lf=36.2944
6 2.963859 0.001174 0.514797
14 1.436099 0.001084 -0.279267
14 -0.909041 1.267031 -0.055434
14 -0.904653 -1.267704 -0.055724
6 -2.082807 -0.002133 0.396194

C2Si32-_070.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.475780551 HF+ZPE=-944.467512 lf=59.1881
6 -0.007846 4.080423 0.000000
14 -0.002450 2.344918 0.000000
6 0.000000 0.619062 0.000000
14 0.001982 -1.084693 0.000000
14 0.003830 -3.274291 0.000000

C2Si32-_072.log mol=C2Si3(2-)
RB3LYP/Aug-CC-pVTZ HF=-944.440913421 HF+ZPE=-944.433938 lf=43.2622
6 0.000000 3.581518 -0.491966
14 0.000000 1.866343 -0.326381
14 0.000000 0.000000 1.074447
14 0.000000 -1.866343 -0.326381
6 0.000000 -3.581518 -0.491966

S5. Table S5. Optimized geometries (in angstrom) of the isomers in Table S2 at the level of B3LYP/aug-cc-pVTZ

C2Si32-_073-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.621254935 HF+ZPE=-944.610871 lf=59.3300
14 0.007937 3.592195 0.000000
6 0.002979 1.799444 0.000000
6 0.000000 0.537553 0.000000
14 -0.003367 -1.229608 0.000000
14 -0.005846 -3.364158 0.000000

C2Si32-_005-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.617223490 HF+ZPE=-944.607044 lf=74.1424
14 2.719459 -1.077429 0.000000
6 1.128417 -0.284441 0.000000
6 0.000000 0.320759 0.000000
14 -1.851452 -0.556527 0.000000
14 -1.351614 1.618390 0.000000

C2Si32-_108-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.608097651 HF+ZPE=-944.596638 lf=115.5569
6 0.658741 -0.912465 0.000000
6 -0.658852 -0.914105 0.000000
14 2.229052 -0.132362 0.000000
14 -2.229005 -0.133320 0.000000
14 0.000000 1.048497 0.000000

C2Si32-_034-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.596669192 HF+ZPE=-944.587025 lf=86.9085
14 -1.470295 -1.118898 -0.170963
14 0.550010 -0.000126 0.611932
14 -1.470199 1.119005 -0.170857
6 2.182551 -0.000107 -0.150017
6 3.395244 0.000151 -0.480245

C2Si32-_136-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.594810453 HF+ZPE=-944.584244 lf=127.6744
14 1.933608 -1.246237 0.000000
6 0.000000 1.066665 0.000000
6 1.035579 0.256814 0.000000
14 -1.674981 1.576574 0.000000
14 -0.702447 -0.897542 0.000000

C2Si32-_001-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.589422521 HF+ZPE=-944.579296 lf=172.3140

6 -1.995558 1.015044 0.000000
6 -1.448270 -0.134678 0.000000
14 0.000000 1.411509 0.000000
14 -0.235629 -1.554748 0.000000
14 1.711555 -0.234060 0.000000

C2Si32-_020-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.588891662 HF+ZPE=-944.578691 lf=135.1195
6 -1.094495 -0.387456 1.289173
6 0.139228 -0.575875 0.886704
14 -1.327147 -0.386475 -0.705574
14 1.579699 -0.552177 -0.245284
14 0.156849 1.351509 0.018339

C2Si32-_025-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.587053826 HF+ZPE=-944.577167 lf=125.6560
6 1.915174 0.041690 0.869801
6 0.929529 0.804921 0.549403
14 0.854594 -0.845131 -0.669616
14 -0.632063 1.312573 -0.336007
14 -1.441690 -0.830274 0.397393

C2Si32-_110-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.586884903 HF+ZPE=-944.577055 lf=100.1420
6 -0.160483 -1.223551 0.146712
14 -1.794485 -0.429360 -0.179594
14 1.758925 0.189455 -0.231318
14 -0.352743 1.411291 0.194822
6 1.066523 -1.509682 0.357498

C2Si32-_006-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.586550983 HF+ZPE=-944.576825 lf=80.9372
14 -1.797721 0.848995 0.000000
6 0.000000 1.232103 0.000000
14 -0.673144 -1.190315 0.000000
6 1.261859 1.069890 0.000000
14 1.930068 -0.645249 0.000000

C2Si32-_041-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.585526098 HF+ZPE=-944.576079 lf=59.9485
6 1.760740 -3.611628 0.000000
6 1.081080 -2.555123 0.000000
14 -0.146000 -1.252036 0.000000
14 0.000000 0.981285 0.000000

14 -1.071922 2.913644 0.000000

C2Si32-_013-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.585293906 HF+ZPE=-944.575480 lf=74.5681
6 -0.040181 0.000000 1.055338
14 1.544466 -0.004276 0.091319
14 -0.475743 -1.297776 -0.485197
14 -0.468087 1.300563 -0.484997
6 -1.361304 0.003474 0.995370

C2Si32-_019-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.583901861 HF+ZPE=-944.574027 lf=101.5824
14 1.678086 -0.853855 0.000000
14 0.000000 0.516428 0.000000
14 -0.597124 -1.857489 0.000000
6 -0.946249 2.018715 0.000000
6 -1.575996 3.102758 0.000000

C2Si32-_010-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.583893240 HF+ZPE=-944.574285 lf=96.3529
6 -0.505595 -2.486850 0.000000
6 -0.737969 -1.235724 0.000000
14 1.401336 -1.441565 0.000000
14 0.000000 0.485626 0.000000
14 -0.868380 2.551327 0.000000

C2Si32-_003-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.583205372 HF+ZPE=-944.573638 lf=67.8604
6 -1.633886 -0.004835 0.000000
14 0.000000 0.646486 0.000000
14 -3.301620 -0.321177 0.000000
6 1.633885 -0.004829 0.000000
14 3.301621 -0.321167 0.000000

C2Si32-_069-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.578731574 HF+ZPE=-944.569569 lf=78.0617
6 1.132829 2.131638 -0.000606
6 1.364496 0.885163 0.000748
14 1.832691 -0.964493 -0.000519
14 -0.335993 -0.281476 0.000889
14 -2.566980 -0.046945 -0.000431

C2Si32-_023-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.571922804 HF+ZPE=-944.562704 lf=54.6864

14 -1.665881 -0.004022 -0.000005
6 -0.042354 -0.000175 -0.967006
6 -0.042375 -0.000510 0.967016
14 0.847324 1.378435 0.000051
14 0.854870 -1.374119 -0.000050

C2Si32-_029-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.566649570 HF+ZPE=-944.557157 lf=124.4203
14 2.175711 -0.000200 -0.000245
6 0.471564 -0.694271 -0.149693
6 0.471864 0.694208 0.150816
14 -1.290265 -1.320969 0.033722
14 -1.289772 1.321197 -0.033958

C2Si32-_014-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.561468948 HF+ZPE=-944.551446 lf=76.9946
14 0.000612 -2.755571 0.000000
6 -0.702383 -1.002974 0.000000
6 0.703124 -1.002716 0.000000
14 0.000000 0.694093 0.000000
14 -0.000929 2.921060 0.000000

C2Si32-_024-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.561462218 HF+ZPE=-944.551926 lf=112.5880
14 -0.000465 1.447121 0.000000
14 1.281728 -0.707079 0.000000
6 -0.000465 -0.035837 1.264510
14 -1.280865 -0.709325 0.000000
6 -0.000465 -0.035837 -1.264510

C2Si32-_079-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.558096800 HF+ZPE=-944.548639 lf=61.6839
14 -0.001122 2.398902 0.000000
6 0.000000 0.657842 0.000000
14 1.179569 -0.856149 0.000000
6 0.000813 -2.258223 0.000000
14 -1.178796 -0.856876 0.000000

C2Si32-_064-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.555669133 HF+ZPE=-944.545899 lf=69.5479
14 2.488612 -0.450251 -0.000072
6 0.916130 0.183207 0.707952
6 0.915985 0.183024 -0.707605
14 -0.698458 0.922832 -0.000105

14 -2.575346 -0.629538 0.000029

C2Si32-_031-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.553483283 HF+ZPE=-944.544059 lf=120.3332
14 -2.262605 -0.000152 0.132177
6 -0.541150 -0.000280 -0.205990
14 0.872978 1.301543 -0.188035
14 0.873558 -1.301395 -0.187979
6 1.745314 0.000290 0.774943

C2Si32-_038-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.551341488 HF+ZPE=-944.542478 lf=48.5383
6 1.233914 0.279242 0.000436
14 2.456107 -0.926095 -0.000097
14 0.000000 1.612840 -0.000131
14 -2.456107 -0.926096 -0.000048
6 -1.233913 0.279244 0.000209

C2Si32-_036-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.511451245 HF+ZPE=-944.503152 lf=48.3082
6 -2.816816 -0.286016 0.935784
14 -1.711700 0.036182 -0.518390
6 0.068433 -0.239398 -0.159861
14 1.201314 1.222712 0.137022
14 1.688264 -1.033717 0.048830

C2Si32-_004-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.511027340 HF+ZPE=-944.502964 lf=64.4283
6 -3.855251 -0.006019 0.000234
14 -2.154417 -0.408834 -0.000105
14 3.228299 -0.264494 0.000047
14 -0.087230 0.662446 -0.000045
6 1.553064 0.031412 0.000006

C2Si32-_016-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.508169293 HF+ZPE=-944.499818 lf=105.7720
14 -1.688287 1.264229 0.000000
6 0.000000 0.891386 0.000000
14 -0.971932 -1.103209 0.000000
14 1.334817 -0.317800 0.000000
6 3.092605 -0.525565 0.000000

C2Si32-_071-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.507795624 HF+ZPE=-944.499733 lf=82.0111

6 -0.739628 -2.691066 0.000000
14 0.155737 -1.175087 0.000000
14 1.781827 0.455171 0.000000
6 0.000000 0.900966 0.000000
14 -1.620581 1.487101 0.000000

C2Si32-_081-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.501473511 HF+ZPE=-944.492506 lf=108.9809
14 2.087723 1.587525 0.000000
14 0.017095 0.463057 0.000000
14 -1.133364 -1.769223 0.000000
6 -1.133364 -0.328251 1.191997
6 -1.133364 -0.328251 -1.191997

C2Si32-_042-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.497629328 HF+ZPE=-944.489779 lf=65.4762
6 0.007775 4.092945 0.000000
14 -0.003007 2.343139 0.000000
6 0.000000 0.625456 0.000000
14 -0.001077 -1.090376 0.000000
14 0.000752 -3.274935 0.000000

C2Si32-_053-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.485355731 HF+ZPE=-944.476819 lf=137.2783
6 -1.219289 0.001338 1.172904
14 -0.354575 1.205709 -0.000021
14 -0.357665 -1.205503 0.000020
14 1.757350 -0.001311 -0.000002
6 -1.219301 0.001240 -1.172899

C2Si32-_021-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.484193355 HF+ZPE=-944.475920 lf=120.0902
6 -2.815177 -0.233814 -0.434573
14 -1.074093 -0.003235 0.106320
6 0.187491 -1.086577 0.897839
14 0.737995 1.422780 0.050363
14 1.462248 -0.853663 -0.355226

C2Si32-_072-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.439748196 HF+ZPE=-944.432902 lf=92.4514
6 0.000000 2.659351 -1.361751
14 0.000000 1.309763 -0.248081
14 0.000000 0.000000 1.663378
14 0.000000 -1.309763 -0.248081

6 0.000000 -2.659351 -1.361751

C2Si32-_105-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.435439139 HF+ZPE=-944.428726 lf=59.8481
6 -3.763201 -0.124424 0.000757
14 -2.028757 -0.311121 -0.000266
14 0.000000 0.728891 -0.000116
14 2.028757 -0.311121 -0.000266
6 3.763200 -0.124424 0.000757

C2Si32-_134-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.410032681 HF+ZPE=-944.403609 lf=59.4186
6 0.000386 2.004152 1.459198
14 0.000386 0.925065 0.000000
14 1.099243 -1.321746 0.000000
6 0.000386 2.004152 -1.459198
14 -1.099961 -1.321164 0.000000

C2Si32-_011-tri.log mol=C2Si3(2-,3)
UB3LYP/Aug-CC-pVTZ HF=-944.395889177 HF+ZPE=-944.388911 lf=54.6101
6 1.591146 -2.476602 0.000000
14 0.000007 -1.581109 0.000000
6 -1.590698 -2.477337 0.000000
14 0.000000 0.793689 0.000000
14 -0.000199 2.910537 0.000000

S6. Table S6. Cartesian coordinates of the isomers in Table S3 at the level of B3LYP/6-31g(d).

"mol"----"Stoichiometry"
"lf"----"lowest frequency(cm-1)"
"HF"----"total energy(a.u.)"
"HF+ZPE"----"zero-point energy corrected total energy(a.u.)"

##
C2Si3-CpMg-cage-1.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.90878951 HF+ZPE=-1731.727784 lf=7.5572
6 0.004210 1.989604 0.942233
14 0.005665 3.759517 0.881093s
14 -1.158466 2.243940 -0.847851
14 1.157404 2.240886 -0.854542
6 0.000576 0.785383 0.320952
6 -4.089036 -1.038815 0.214778
6 -3.594198 -1.523597 -1.027535
6 -2.496357 -2.391903 -0.755885
6 -2.318637 -2.446785 0.655708
6 -3.298338 -1.607161 1.256247
1 -4.933978 -0.373745 0.347333
1 -3.997044 -1.293280 -2.006564
1 -1.929167 -2.949341 -1.492135
1 -1.581712 -3.041427 1.182320
1 -3.443101 -1.456724 2.319611
6 4.091944 -1.042227 0.176916
6 3.566392 -1.553281 -1.042024
6 2.472927 -2.411692 -0.724801
6 2.328393 -2.433748 0.691344
6 3.324379 -1.583918 1.249361
1 4.941597 -0.377054 0.274220
1 3.947287 -1.347397 -2.035187
1 1.886944 -2.983861 -1.434563
1 1.601778 -3.012872 1.248678
1 3.494529 -1.409676 2.305303
12 1.897488 -0.235446 -0.041895
12 -1.897913 -0.233435 -0.037655

CpMg-020-d2-t4.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.90588749 HF+ZPE=-1731.725001 lf=3.1288
6 1.065874 1.083167 0.010284
6 0.441051 2.305554 -0.000127
14 -0.474391 1.034264 -1.319293

14 -1.089597 3.189861 -0.011269
14 -0.483751 1.049606 1.327841
6 -4.384038 -1.012636 -1.066732
6 -3.577344 -2.169939 -0.880350
6 -3.432080 -2.384652 0.520404
6 -4.151122 -1.360672 1.199063
6 -4.737533 -0.510878 0.218766
1 -4.696845 -0.601257 -2.019097
1 -3.171355 -2.795672 -1.666454
1 -2.899685 -3.204833 0.987571
1 -4.254678 -1.259440 2.272896
1 -5.369718 0.346795 0.415984
6 4.252800 -1.410977 -1.152153
6 3.795888 -2.099237 0.009368
6 4.275554 -1.397922 1.153879
6 5.026956 -0.275862 0.699471
6 5.012807 -0.283977 -0.725577
1 4.079114 -1.710093 -2.178939
1 3.217905 -3.015668 0.020237
1 4.122898 -1.685680 2.187234
1 5.546715 0.438488 1.326821
1 5.519639 0.423331 -1.371217
12 2.816121 0.016436 0.008162
12 -2.395998 -0.321438 0.003946

CpMg-015-d1-d2.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.89576035 HF+ZPE=-1731.714966 lf=4.3669
14 1.141966 2.547823 -0.007364
6 -0.000431 1.063219 -0.015055
14 -1.141853 2.548654 -0.008495
6 -0.000273 -0.340072 -0.024624
14 -0.000307 -2.038668 -0.039519
6 -4.276240 -0.277591 -1.123303
6 -3.848358 -1.577715 -0.722476
6 -3.820790 -1.612609 0.697716
6 -4.231004 -0.334108 1.178138
6 -4.522099 0.485215 0.051974
1 -4.432098 0.055607 -2.142699
1 -3.612826 -2.402986 -1.383701
1 -3.559477 -2.468739 1.308033
1 -4.346880 -0.051511 2.217963
1 -4.870363 1.509976 0.083881
6 4.276104 -0.275440 -1.123222
6 3.849497 -1.576467 -0.724043

6 3.822135 -1.613225 0.696123
6 4.231118 -0.334907 1.178133
6 4.521345 0.486056 0.053001
1 4.431367 0.059236 -2.142231
1 3.614872 -2.401130 -1.386359
1 3.561769 -2.470401 1.305389
1 4.346885 -0.053597 2.218321
1 4.868439 1.511177 0.086186
12 2.212376 -0.027958 -0.004682
12 -2.212791 -0.026299 -0.005623

C2Si3-CpMg-planar-1.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.89571211 HF+ZPE=-1731.714912 lf=4.5476
14 -0.015966 -2.042355 -0.019820
6 -0.003004 -0.343498 -0.011142
6 0.006107 1.060147 -0.006371
14 -1.134434 2.547494 -0.007572
14 1.149661 2.542732 -0.001209
6 -4.275877 -0.277817 -1.131175
6 -3.843899 -1.575360 -0.726509
6 -3.821660 -1.607709 0.693735
6 -4.239460 -0.330369 1.170429
6 -4.529856 0.485697 0.041914
1 -4.429728 0.053291 -2.151574
1 -3.602533 -2.400634 -1.385574
1 -3.559191 -2.461672 1.306482
1 -4.360905 -0.046521 2.209271
1 -4.882998 1.508936 0.070551
6 3.794935 -1.786249 -0.257666
6 4.117906 -0.764603 -1.196415
6 4.485500 0.402211 -0.466717
6 4.376709 0.106998 0.919365
6 3.948706 -1.247131 1.049243
1 3.505453 -2.802053 -0.497259
1 4.130427 -0.871809 -2.274846
1 4.800673 1.346881 -0.892358
1 4.606935 0.783746 1.733550
1 3.805012 -1.783269 1.979980
12 2.208784 -0.047385 -0.007031
12 -2.217071 -0.013531 -0.007133

CpMg-023-d2-t2.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88997558 HF+ZPE=-1731.709931 lf=8.1222
14 -0.003672 1.750371 -0.810374

6 -0.743150 0.002528 -1.092922
6 0.742759 0.007774 -1.092329
14 0.002484 -1.741768 -0.819107
14 0.000168 -0.000418 1.004640
6 4.661145 0.770656 -0.629683
6 4.489624 1.125238 0.740483
6 4.399764 -0.076873 1.497950
6 4.509586 -1.174263 0.597194
6 4.673758 -0.649624 -0.718158
1 4.788856 1.460644 -1.455404
1 4.467513 2.132397 1.139814
1 4.282506 -0.144671 2.572852
1 4.506475 -2.223495 0.868315
1 4.811430 -1.229746 -1.622940
6 -4.666393 -0.697507 -0.689302
6 -4.498975 -1.162385 0.648014
6 -4.500203 1.141262 0.690093
6 -4.666844 0.725069 -0.663542
1 -4.797174 -1.318178 -1.567848
1 -4.486282 -2.198542 0.965095
1 -4.799260 1.377353 -1.518613
6 -4.400236 -0.025555 1.499630
1 -4.284196 -0.045309 2.576635
1 -4.489126 2.165276 1.044508
12 2.551454 -0.003545 0.041236
12 -2.550744 0.002858 0.043829

CpMg-015-d1-s1.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88957608 HF+ZPE=-1731.708618 lf=12.0635
14 -0.438233 -0.353843 -0.009054
6 0.372412 1.279611 -0.002400
14 -1.304919 2.004692 -0.000324
6 1.629391 1.854374 -0.000366
14 3.038272 2.800252 0.002168
6 4.431444 -1.473067 -1.148124
6 3.225534 -2.097369 -0.716444
6 3.218332 -2.099755 0.709072
6 4.419750 -1.476861 1.155030
6 5.168418 -1.092122 0.007844
1 4.745485 -1.338571 -2.176464
1 2.463127 -2.526185 -1.355330
1 2.449520 -2.530701 1.338772
1 4.723339 -1.345856 2.186955
1 6.136154 -0.605121 0.013546

6 -5.397214 0.407862 -0.174729
6 -5.156704 -0.205161 1.087353
6 -4.656213 -1.519075 0.850464
6 -4.585766 -1.715826 -0.556911
6 -5.040636 -0.523526 -1.191754
1 -5.803189 1.399732 -0.333602
1 -5.355380 0.235358 2.057214
1 -4.403086 -2.250358 1.608882
1 -4.267235 -2.622255 -1.057754
1 -5.138232 -0.368017 -2.259689
12 3.130483 0.123967 -0.000462
12 -3.085039 0.009536 -0.002521

C2Si3-CpMg-planar-C-C.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88709457 HF+ZPE=-1731.706369 lf=12.1483
6 0.526164 -1.233934 -0.044722
6 -0.687731 -1.506258 -0.043470
14 -3.949271 0.041872 0.045304
14 -2.487014 -1.724968 -0.029914
14 -4.640365 -2.254453 0.011295
6 4.518657 -0.559407 -1.191427
6 4.357318 0.521000 -0.275257
6 4.408414 -0.011343 1.046382
6 4.602740 -1.420397 0.946431
6 4.671140 -1.758643 -0.435916
1 4.557522 -0.478087 -2.271171
1 4.252397 1.567465 -0.535467
1 4.351141 0.559468 1.965531
1 4.714571 -2.108071 1.776210
1 4.843209 -2.748700 -0.841093
6 0.422077 2.301959 0.686163
6 -0.804446 2.866431 1.144723
6 -1.574394 3.225053 0.007096
6 -0.840341 2.867797 -1.154618
6 0.399697 2.303053 -0.735632
1 1.242643 1.978096 1.316542
1 -1.081231 3.029349 2.179679
1 -2.561645 3.669126 0.023122
1 -1.149890 3.030868 -2.180215
1 1.198302 1.976140 -1.391967
12 2.546715 -0.911670 -0.012419
12 -1.320855 0.834849 0.002980

CpMg-001-t1-s4.log mol=C12H10Mg2Si3

RB3LYP/6-31G(d) HF=-1731.88692543 HF+ZPE=-1731.706417 lf=15.6245
6 -0.147457 -0.937203 -0.003389
6 1.028482 -1.383286 -0.007238
14 2.612751 -2.365115 -0.011098
14 3.407892 0.004131 0.010771
14 4.862397 -1.642797 0.004647
6 -0.805424 2.584170 0.694087
6 -0.788247 2.586855 -0.724624
6 0.474636 3.094117 -1.149488
6 1.228101 3.418989 0.010784
6 0.446891 3.089463 1.151374
1 -1.636520 2.289161 1.324939
1 -1.603240 2.293147 -1.376697
1 0.784146 3.253006 -2.175845
1 2.227196 3.837063 0.023675
1 0.731445 3.244811 2.185474
6 -4.222759 0.200592 -0.123525
6 -4.190901 -0.753432 -1.182366
6 -4.144419 -2.054375 -0.601489
6 -4.145531 -1.905063 0.814638
6 -4.192915 -0.511410 1.111171
1 -4.296327 1.275652 -0.236555
1 -4.235812 -0.530725 -2.241845
1 -4.139923 -2.993046 -1.142669
1 -4.142078 -2.710234 1.539643
1 -4.240019 -0.072576 2.100762
12 -2.191623 -0.928455 -0.002907
12 0.937108 1.060969 0.002825

CpMg-001-d1-t2.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88632847 HF+ZPE=-1731.705404 lf=12.4377
6 1.177352 -0.900799 -0.009443
6 -0.000739 -1.281580 -0.007918
14 -3.917227 -1.241601 0.006018
14 -1.698931 -1.871700 -0.003380
14 -3.188981 -3.517034 0.001166
6 5.360451 -1.123459 -0.378442
6 5.105156 0.006953 -1.208134
6 4.844789 1.124200 -0.362179
6 4.938647 0.683930 0.990101
6 5.257637 -0.705154 0.980003
1 5.619852 -2.118353 -0.720271
1 5.137970 0.021996 -2.291028
1 4.645853 2.137821 -0.689316

1 4.822240 1.303884 1.871075
1 5.424661 -1.326505 1.851758
6 -2.982313 3.083978 -0.721370
6 -1.655340 2.785612 -1.148700
6 -0.849239 2.611720 0.012233
6 -1.678981 2.792642 1.155373
6 -2.996813 3.088399 0.699178
1 -3.827834 3.289647 -1.366838
1 -1.312149 2.738135 -2.175503
1 0.208891 2.382328 0.023714
1 -1.356933 2.751470 2.189277
1 -3.855455 3.297509 1.325934
12 3.164129 -0.449570 -0.006903
12 -2.444027 0.895245 0.000546

CpMg-023-d1-t1.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88524230 HF+ZPE=-1731.705419 lf=4.7659
14 0.449390 1.899818 -1.740083
6 -0.062293 0.835823 0.001424
6 0.960233 2.149308 0.000171
14 0.445580 1.905496 1.739977
14 -1.051551 2.645354 -0.002991
6 -2.562987 -2.398241 0.067840
6 -3.152707 -1.718568 1.171969
6 -4.026310 -0.717163 0.656700
6 -3.974156 -0.777099 -0.765606
6 -3.068561 -1.815951 -1.129539
1 -1.872731 -3.231512 0.128276
1 -2.992686 -1.945999 2.219346
1 -4.644571 -0.048068 1.243230
1 -4.546476 -0.162105 -1.449906
1 -2.833984 -2.130572 -2.139641
6 3.065615 -1.740676 -1.167133
6 3.954258 -0.743727 -0.670866
6 3.915571 -0.789539 0.753077
6 3.003016 -1.814861 1.135326
6 2.478703 -2.401961 -0.051075
1 2.889170 -1.972622 -2.210825
1 4.573221 -0.086316 -1.269728
1 4.500685 -0.173704 1.425630
1 2.771289 -2.113419 2.150927
1 1.776160 -3.225890 -0.096976
12 -1.853530 -0.162074 -0.000143
12 1.802677 -0.139861 0.002584

CpMg-001-d1-t5.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88427783 HF+ZPE=-1731.703284 lf=8.7160
6 -2.819922 -0.021918 0.006790
6 -1.585630 -0.022275 0.003369
14 1.923355 -1.389432 -0.033684
14 0.201090 -0.018307 0.003399
14 1.912894 1.365752 -0.034589
6 6.228525 -1.177020 -0.200200
6 6.202478 -0.565234 1.083719
6 6.196058 0.849179 0.897879
6 6.214761 1.108757 -0.499632
6 6.228669 -0.143674 -1.180499
1 6.256725 -2.241863 -0.397695
1 6.221536 -1.082536 2.035721
1 6.202690 1.594968 1.683879
1 6.232141 2.086951 -0.965089
1 6.276823 -0.284529 -2.253931
6 -6.834033 0.874561 -0.849908
6 -6.834121 1.092055 0.558489
6 -6.849421 -0.180253 1.200751
6 -6.858812 -1.184164 0.189081
6 -6.849014 -0.532237 -1.078272
1 -6.850762 1.643665 -1.612878
1 -6.851670 2.055511 1.053878
1 -6.881965 -0.353469 2.269822
1 -6.899417 -2.254204 0.354382
1 -6.880526 -1.019964 -2.045276
12 -4.857599 -0.009239 0.008469
12 4.192136 -0.002708 -0.008801

CpMg-002-s1-t3.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88424290 HF+ZPE=-1731.704254 lf=16.1154
6 -0.002652 -1.330521 1.167531
14 -0.007054 -2.765032 0.260533
6 0.002586 1.358395 1.149456
14 0.005486 2.782094 0.225711
14 0.002209 0.021699 2.451126
6 2.963680 -0.698737 -1.704432
6 2.990842 0.729644 -1.670725
6 3.603854 1.126147 -0.452450
6 3.945984 -0.049767 0.273569
6 3.561343 -1.175600 -0.507279
1 2.597321 -1.308444 -2.521953

1 2.646719 1.390843 -2.457277
1 3.789397 2.145454 -0.135123
1 4.455035 -0.081918 1.229843
1 3.707919 -2.215266 -0.239542
6 -2.973193 -0.735101 -1.678959
6 -2.977248 0.693729 -1.696449
6 -3.586047 1.143555 -0.494381
6 -3.947183 0.000027 0.272810
6 -3.579118 -1.159133 -0.466591
1 -2.613611 -1.379122 -2.472813
1 -2.623153 1.320986 -2.506048
1 -3.756333 2.176391 -0.214426
1 -4.458172 0.010404 1.228539
1 -3.742025 -2.185805 -0.160851
12 1.573336 0.002012 0.080329
12 -1.575765 0.011987 0.084160

CpMg-020-d2-t3.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88283633 HF+ZPE=-1731.702066 lf=9.4820
6 -1.378430 -0.045292 1.025728
6 -0.076297 -0.033717 0.994100
14 -0.820101 -1.116837 -0.841500
14 1.148096 0.127099 -0.356915
14 -0.851832 1.392204 -0.581854
6 5.786942 0.293516 -0.965562
6 5.674711 -1.058231 -0.527507
6 5.522747 -1.051012 0.889352
6 5.541305 0.305751 1.327405
6 5.705390 1.136440 0.180846
1 5.945575 0.620617 -1.986258
1 5.730068 -1.938342 -1.156973
1 5.442743 -1.924200 1.525697
1 5.479865 0.643904 2.354885
1 5.789313 2.216624 0.184301
6 -5.333288 -1.160657 0.637338
6 -5.228170 -0.907812 -0.760906
6 -5.238875 0.504005 -0.954138
6 -5.350706 1.121722 0.325895
6 -5.410603 0.092238 1.306817
1 -5.372020 -2.137029 1.105806
1 -5.174613 -1.656769 -1.541899
1 -5.198718 1.016633 -1.907768
1 -5.409938 2.187040 0.514882
1 -5.514580 0.237440 2.375621

12 -3.306113 -0.028430 0.241129
12 3.666752 0.021584 -0.026189

CpMg-002-s1-t1.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88109520 HF+ZPE=-1731.700930 lf=6.3365
6 -0.311238 -0.276342 -0.035630
14 -0.428107 -1.971679 -0.063236
6 1.400736 2.080728 -0.014603
14 2.773599 3.061104 -0.000590
14 -0.314252 1.588113 -0.030853
6 -4.380933 -0.957973 0.892240
6 -4.557512 0.441701 1.099091
6 -4.666626 1.064040 -0.176722
6 -4.547447 0.052560 -1.172120
6 -4.376311 -1.197998 -0.509723
1 -4.296117 -1.710447 1.667311
1 -4.632534 0.939895 2.058408
1 -4.822748 2.120626 -0.357876
1 -4.619508 0.201638 -2.243083
1 -4.286232 -2.165382 -0.989264
6 3.049329 -2.079045 0.713654
6 3.870715 -1.015545 1.183607
6 4.420778 -0.354331 0.052858
6 3.927624 -0.992524 -1.116558
6 3.084038 -2.064554 -0.709200
1 2.528837 -2.801226 1.331595
1 4.074987 -0.780261 2.221718
1 5.103162 0.486435 0.078180
1 4.181831 -0.736009 -2.138481
1 2.594639 -2.773647 -1.366518
12 2.032468 -0.030054 -0.002942
12 -2.511017 0.157432 -0.011878

C2Si3-CpMg-1-ptSi.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.88082321 HF+ZPE=-1731.700342 lf=5.0456
14 -0.020040 2.174505 -0.371688
14 -0.001363 0.026501 -1.585237
6 -0.009459 0.669282 0.618707
14 0.021519 -2.143310 -0.402372
6 0.006133 -0.652058 0.612079
6 -4.025205 -1.139744 0.842591
6 -3.870123 0.079324 1.563771
6 -4.120740 1.155782 0.664648
6 -4.429175 0.602019 -0.609812

6 -4.369612 -0.815795 -0.500572
1 -3.925182 -2.138186 1.251565
1 -3.634267 0.170167 2.617517
1 -4.103630 2.210269 0.913488
1 -4.683025 1.161924 -1.502101
1 -4.573570 -1.525143 -1.293797
6 3.939423 -0.747129 1.319931
6 3.890738 0.676076 1.368824
6 4.217306 1.171374 0.073632
6 4.466877 0.055539 -0.774147
6 4.295984 -1.129477 -0.004905
1 3.767332 -1.418582 2.152851
1 3.674896 1.275978 2.244995
1 4.286988 2.214752 -0.210303
1 4.756040 0.101241 -1.817389
1 4.435660 -2.144149 -0.358495
12 2.200941 -0.037014 -0.091164
12 -2.197253 0.014750 -0.076891

CpMg-015-d1-t1.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.87578275 HF+ZPE=-1731.694873 lf=12.4509
14 -0.323058 2.260593 -0.002040
6 1.478497 2.036196 -0.000617
14 1.182760 3.924062 0.001369
6 2.635591 1.314266 -0.000357
14 4.232405 0.705187 0.000363
6 -3.789519 -0.755851 -1.150960
6 -3.349027 -1.465589 0.004117
6 -3.791264 -0.749245 1.154436
6 -4.506529 0.400391 0.709517
6 -4.505453 0.396314 -0.713715
1 -3.643562 -1.061398 -2.180244
1 -2.805090 -2.402414 0.007178
1 -3.646806 -1.048867 2.185671
1 -4.992189 1.132486 1.343617
1 -4.990164 1.124737 -1.352749
6 0.414242 -2.313528 -0.712723
6 1.611548 -2.947614 -1.150925
6 2.347921 -3.339813 -0.000306
6 1.612981 -2.947213 1.151081
6 0.415146 -2.313276 0.714187
1 -0.377344 -1.945699 -1.354804
1 1.897198 -3.122287 -2.181321
1 3.302624 -3.851786 -0.000807

1 1.899989 -3.121417 2.181179
1 -0.375557 -1.945039 1.357121
12 -2.279772 0.613911 -0.001077
12 2.196155 -0.956105 -0.000835

CpMg-009-d1-d3.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.87568264 HF+ZPE=-1731.694725 lf=20.7460
14 -2.436479 1.979417 -1.360445
14 -0.111058 2.151529 -0.749674
6 -1.932112 1.931019 0.417923
14 0.806029 2.435709 1.465165
6 -0.943623 2.092665 1.238642
6 2.849944 -1.399582 -1.329537
6 3.679532 -0.247367 -1.224903
6 4.053152 -0.095745 0.139030
6 3.453926 -1.152199 0.880647
6 2.709875 -1.959746 -0.027342
1 2.429143 -1.799139 -2.244549
1 3.995143 0.385423 -2.046005
1 4.697798 0.676752 0.540876
1 3.573498 -1.331727 1.942502
1 2.173794 -2.868002 0.221233
6 -1.178354 -2.616569 -0.343442
6 -1.073637 -2.154182 1.004584
6 -2.389754 -1.865962 1.471358
6 -3.299109 -2.138499 0.413721
6 -2.550414 -2.602986 -0.705756
1 -0.357835 -2.947226 -0.968388
1 -0.168651 -2.114539 1.599202
1 -2.649542 -1.518776 2.464061
1 -4.376565 -2.032440 0.458883
1 -2.958897 -2.905465 -1.662540
12 -1.885677 -0.355181 -0.255247
12 1.697899 0.169922 0.014791

CpMg-009-d1-t3.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.87437513 HF+ZPE=-1731.693589 lf=15.0942
14 2.462230 -1.888917 -1.492129
14 0.185193 -2.129243 -0.660996
6 2.112089 -1.862207 0.298203
14 -0.497152 -2.145493 1.700055
6 1.214634 -1.936717 1.241338
6 2.118944 2.010712 1.458934
6 3.152676 2.094834 0.487040

6 2.567315 2.493989 -0.747827
6 1.174012 2.660369 -0.543686
6 0.889191 2.357055 0.821762
1 2.245544 1.759983 2.505467
1 4.204538 1.900381 0.660513
1 3.092792 2.647262 -1.682650
1 0.454287 2.985493 -1.285275
1 -0.068923 2.462868 1.317696
6 -3.022691 1.387341 -1.215409
6 -3.050925 1.739035 0.165460
6 -3.612627 0.645668 0.885036
6 -3.930282 -0.381618 -0.046985
6 -3.566839 0.076853 -1.344881
1 -2.688622 2.023481 -2.026357
1 -2.750459 2.691371 0.586384
1 -3.787772 0.609370 1.953623
1 -4.383751 -1.336883 0.189688
1 -3.704849 -0.463621 -2.273734
12 -1.579380 -0.074411 -0.077286
12 1.663584 0.349375 -0.119071

CpMg-026-s1-t1.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.87409076 HF+ZPE=-1731.693750 lf=14.8899
6 0.637037 -1.290718 -0.007301
14 -0.009686 0.603727 -0.005338
6 -0.643615 -1.294069 -0.008334
14 1.223927 2.481762 0.000653
14 -1.165942 2.528463 0.000322
6 -4.490293 -1.446191 0.987340
6 -4.690295 -0.032493 0.977873
6 -4.760042 0.391413 -0.379180
6 -4.593687 -0.757792 -1.207595
6 -4.435650 -1.891821 -0.359812
1 -4.420760 -2.072715 1.868758
1 -4.808925 0.601316 1.848570
1 -4.926000 1.405560 -0.720656
1 -4.631133 -0.771680 -2.290601
1 -4.300514 -2.916012 -0.686273
6 4.743754 0.204235 0.705853
6 4.744885 0.191763 -0.716714
6 4.514747 -1.150546 -1.144821
6 4.380139 -1.964421 0.013132
6 4.512520 -1.130239 1.157030
1 4.914161 1.069976 1.334145

1 4.917089 1.046220 -1.359829
1 4.489332 -1.494694 -2.172148
1 4.203644 -3.033255 0.022355
1 4.485397 -1.456285 2.190208
12 -2.611564 -0.431067 -0.004510
12 2.601941 -0.397974 -0.002014

CpMg-015-d1-s6.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.87056101 HF+ZPE=-1731.690186 lf=22.3607
14 -3.852639 0.389606 0.927277
6 -3.064973 -1.001314 -0.117501
14 -4.842030 -1.471922 0.030222
6 -1.820055 -1.259533 -0.568154
14 -0.257083 -1.562216 -1.172381
6 1.283808 2.166460 0.697046
6 -0.048560 2.638321 0.764055
6 -0.505292 2.842044 -0.586703
6 0.536735 2.471815 -1.459758
6 1.649134 2.070101 -0.679729
1 1.941445 2.022992 1.546788
1 -0.564694 2.953414 1.665285
1 -1.440445 3.315361 -0.873231
1 0.505031 2.521701 -2.541369
1 2.656705 1.918756 -1.058568
6 3.008932 -2.085196 0.952570
6 3.381951 -0.875133 1.607979
6 4.114196 -0.082666 0.682046
6 4.179861 -0.793701 -0.549550
6 3.503297 -2.034759 -0.376504
1 2.462345 -2.907648 1.398045
1 3.188266 -0.628534 2.645566
1 4.565337 0.881605 0.885846
1 4.703527 -0.473708 -1.443237
1 3.392430 -2.808484 -1.126501
12 1.889187 -0.290586 -0.152406
12 -1.339154 0.781367 0.128652

CpMg-001-d2-t2.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.86807576 HF+ZPE=-1731.687898 lf=13.3463
6 -0.476340 -0.457011 -1.013892
6 0.561402 -1.159195 -1.288548
14 -0.050892 -1.684582 0.734521
14 1.894559 -2.458529 -1.157376
14 2.201919 -2.143909 1.215800

6 1.695531 2.580954 0.500004
6 2.840561 2.129677 1.222338
6 3.822733 1.726855 0.280649
6 3.290980 1.927879 -1.026700
6 1.980102 2.463362 -0.890307
1 0.792390 2.994655 0.933520
1 2.946566 2.113750 2.300488
1 4.809352 1.344746 0.514022
1 3.809257 1.743796 -1.960393
1 1.321000 2.746957 -1.702166
6 -3.733450 1.656148 0.394528
6 -3.957539 0.591075 1.317486
6 -4.524717 -0.500516 0.598915
6 -4.648873 -0.110654 -0.767122
6 -4.163329 1.222613 -0.890828
1 -3.340792 2.636363 0.637688
1 -3.764994 0.620137 2.383286
1 -4.834402 -1.448505 1.021967
1 -5.075642 -0.709460 -1.563082
1 -4.143831 1.810613 -1.800662
12 -2.377200 -0.145587 -0.224019
12 1.937244 0.290431 0.016933

CpMg-020-d4-t3.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.86632571 HF+ZPE=-1731.686222 lf=9.7116
6 0.486482 -2.137204 0.013738
6 0.853552 -0.812765 -0.005618
14 -0.641460 -1.213067 -1.333867
14 0.178078 0.894571 -0.023404
14 -0.627894 -1.177969 1.348712
6 -4.543424 0.831879 -1.193076
6 -5.006873 -0.361198 -0.570053
6 -4.938565 -0.176255 0.840710
6 -4.432244 1.130763 1.089262
6 -4.186686 1.753801 -0.168043
1 -4.495651 1.016159 -2.259797
1 -5.376468 -1.243325 -1.079418
1 -5.247899 -0.892716 1.592427
1 -4.290202 1.584074 2.063183
1 -3.823477 2.763587 -0.318359
6 4.828464 0.160270 -1.180903
6 4.734595 1.458135 -0.597141
6 4.731874 1.304500 0.818664
6 4.825306 -0.088185 1.110948

6 4.887839 -0.794087 -0.124473
1 4.885498 -0.058798 -2.240487
1 4.698980 2.397535 -1.135414
1 4.693897 2.106882 1.545566
1 4.873038 -0.530169 2.099039
1 4.982743 -1.866948 -0.240396
12 -2.732978 -0.093057 0.004719
12 2.810936 0.264417 -0.013937

CpMg-073-s1-t2.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.84491599 HF+ZPE=-1731.664672 lf=10.7274
14 4.215933 3.196917 0.002167
6 2.718446 2.349430 -0.000079
6 1.625520 1.659216 -0.004119
14 -0.112997 1.263375 -0.004197
14 -0.734792 -0.911024 -0.050624
6 -5.306905 -0.553222 0.987689
6 -5.011419 0.840379 1.004542
6 -4.937179 1.290772 -0.344975
6 -5.186273 0.174948 -1.195289
6 -5.414793 -0.963904 -0.371145
1 -5.454875 -1.182967 1.856929
1 -4.897151 1.456800 1.888252
1 -4.757416 2.309586 -0.666951
1 -5.228809 0.196681 -2.277753
1 -5.659103 -1.961228 -0.717266
6 4.140453 -1.132150 0.665352
6 3.320529 -2.176678 1.184367
6 2.783015 -2.900567 0.084062
6 3.255173 -2.297125 -1.113428
6 4.098833 -1.204890 -0.753125
1 4.709945 -0.418636 1.248379
1 3.167542 -2.405041 2.232728
1 2.124062 -3.757880 0.147386
1 3.042426 -2.631754 -2.122023
1 4.634974 -0.559832 -1.438783
12 -3.197626 -0.248142 -0.015196
12 1.918626 -0.689585 -0.007876

CpMg-011-s1-d8.log mol=C12H10Mg2Si3
RB3LYP/6-31G(d) HF=-1731.84421584 HF+ZPE=-1731.664695 lf=4.9166
6 -0.156451 0.181976 -1.838994
14 0.917306 2.912456 -0.778333
6 0.364289 1.293309 -1.580336

14 0.019577 1.863666 1.156334
14 0.005157 0.060323 2.358192
6 3.844234 -0.353476 -0.709338
6 3.740331 -0.546978 0.697820
6 2.990285 -1.728822 0.925629
6 2.632992 -2.276213 -0.350619
6 3.172198 -1.429942 -1.354325
1 4.383341 0.446126 -1.203865
1 4.167317 0.092085 1.461475
1 2.769168 -2.170587 1.889488
1 2.095252 -3.202297 -0.516827
1 3.080710 -1.574153 -2.423937
6 -4.011666 0.308616 -0.509092
6 -3.767713 -0.128271 0.825639
6 -3.322203 -1.477136 0.771422
6 -3.299579 -1.878425 -0.598478
6 -3.733334 -0.779484 -1.385070
1 -4.393503 1.280054 -0.800948
1 -3.913632 0.459215 1.723877
1 -3.082676 -2.103424 1.622347
1 -3.031111 -2.860556 -0.969521
1 -3.828762 -0.768060 -2.464161
12 1.523707 -0.219169 -0.162264
12 -1.703288 -0.149127 -0.336918