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Supplementary Material

A density functional theory investigation of tandem radical cyclization of 1-[2-yl-3-(2-methoxyphenyl)-prop-2-enyl]-6-oxo-1,6-dihydropyridine-2-carbonitrile

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Contents

1. Assignment of transition states and IRC computations

In computations, all transition states were located at the BH*and*HLYP/6-311++G(d,p)~LANL2DZ (LANL2DZ only for the Sn and I atoms, and the same below) level of theory. Further, we also conducted intrinsic reaction coordinates (IRC) calculations to correlate these transition state with the forward and reverse structures. However, the IRC computations are very expensive at the BH*and*HLYP/6-311++G(d,p)~LANL2DZ level of theory, and we only completed several key cyclization transition states at this level. For all transition states, we reoptimized their structures and performed IRC computations at the low-cost BH*and*HLYP/6-31G(d,p)~LANL2DZ level of theory and without the consideration of solvent effects. For the mentioned several cyclization transition states, the results is in good agreement with each other. Thus, the forward and reverse structures connected by a transition state can be reasonably assigned by the low-cost computations.

However, using the Gaussian09 program package, we did not obtain the normal termination for some special transition states. Such a question was frequently found for the Gaussian09 program package. Thus, we reoptimized those structures and conducted IRC computations using the Gaussian03 program. For those transition states, the motion of imaginary vibrational mode optimized by the Gaussian09 package agrees well with the Gaussian03-optimized result. In fact, the computations for many similar systems demonstrate that this kind of cyclization reactions have very simple and readily assigned transition states relative to some inorganic and hypervalent molecules.

2. Selection of the used functional

For the C- and N-centered radicals, their intermolecular or intramolecular additions onto unsaturated groups, such as CC double bond, CC and CN triple bonds, can be well described by the BH*and*HLYP and B3LYP methods, and the former has a better convergence than the latter. In two previous reports, (*Comput. Theor. Chem.*, **2013**, *1005*, 75; **2013**, *1025*, 52), a comparison has been done for the two methods, and the results indicate that they have a good agreement with each other in investigating the intermolecular or intramolecular additions of C- and N-centered radicals onto unsaturated groups. Based on a better convergence of BH*and*HLYP than B3LYP, we selected the BH*and*HLYP functional in the present study. In several important investigations (*J. Org. Chem.* **2008**, *73*, 427; **2008**, *73*, 5821; **2006**, *71*, 4040; **2008**, *73*, 1413. *Acc. Chem. Res.* **2007**, *40*, 303. *J. Phys. Chem. A* **2006**, *110*, 2195. *Aust. J. Chem.* **2007**, *60*, 420.), the authors also used the BH*and*HLYP functional to predict reaction mechanism and relevant energies. Thus, we would like to employ the BH*and*HLYP functional to investigate the present reactions.

Table AP1. Calculated Gibbs free energies (G, in *a.u.*, 298.15 K), enthalpies (H, in *a.u.*, 298.15 K), relative Gibbs free energies (ΔG, in kcal/mol, 298.15 K), and relative enthalpies (ΔH, in kcal/mol, 298.15 K) of stationary points in the investigated tandem radical cyclization at the BH*and*HLYP/6-311++G(d,p) level of theory.

Species	H	ΔH	G	ΔG
2a	–761.876508	–	–761.927670	–
·OCH3	–114.989557	–	–115.016281	–
2a + ·OCH3	–876.866065	–49.17	–876.943951	–55.48
3b	–876.787713	0.00	–876.855542	0.00
4b′	–876.830011	–26.54	–876.892477	–23.18
4b	–876.832567	–28.15	–876.892305	–23.07
5b	–876.815931	–17.71	–876.875925	–12.79
6b	–876.844313	–35.52	–876.903474	–30.08
7b	–876.838072	–31.60	–876.896986	–26.01
9	–876.805991	–11.47	–876.868813	–8.33
10	–876.789149	–0.90	–876.847916	4.79
11	–876.797198	–5.95	–876.855575	–0.02
12	–876.787100	0.38	–876.845808	6.11
13	–876.791245	–2.22	–876.849807	3.60
14	–876.844707	–35.76	–876.903970	–30.39
15	–876.839781	–32.67	–876.898839	–27.17
16	–876.840432	–33.08	–876.900896	–28.46
17	–876.820793	–20.76	–876.880746	–15.82
18	–876.831099	–27.23	–876.890363	–21.85
19	–876.839765	–32.66	–876.898925	–27.22
20	–876.827684	–25.08	–876.887015	–19.75
21	–876.827630	–25.05	–876.887441	–20.02
TS4	–876.778874	5.55	–876.843305	7.68
TS5	–876.757096	19.21	–876.821033	21.65
TS6	–876.808724	–13.18	–876.868004	–7.82
TS7	–876.796700	–5.64	–876.856550	–0.63
TS8	–876.797236	–5.98	–876.856711	–0.73
TS9	–876.827227	–24.80	–876.886111	–19.18
TS10	–876.778801	5.59	–876.837770	11.15
TS11	–876.784004	2.33	–876.842854	7.96
TS12	–876.829896	–26.47	–876.890669	–22.04
TS13	–876.775750	7.51	–876.834251	13.36
TS14	–876.783026	2.94	–876.841392	8.88
TS15	–876.783137	2.87	–876.841430	8.86
TS16	–876.790122	–1.51	–876.848364	4.50
TS17	–876.784361	2.10	–876.841668	8.71

TS18	–876.779960	4.87	–876.838369	10.78
TS19	–876.774771	8.12	–876.833042	14.12
TS20	–876.783970	2.35	–876.842145	8.41
TS21	–876.786300	0.89	–876.844299	7.06
TS22	–876.790184	–1.55	–876.848193	4.61
TS23	–876.828868	–25.83	–876.888134	–20.45
TS24	–876.785264	1.54	–876.843741	7.41
TS25	–876.783761	2.48	–876.841806	8.62

Table AP2. Calculated enthalpies (H, in *a.u.*, 298.15 K), Gibbs free energies (G, in *a.u.*, 298.15 K), relative enthalpies (ΔG, in kcal/mol, 298.15 K), and relative Gibbs free energies (ΔG, in kcal/mol, 298.15 K) of reactants, products, and transition states on the deiodination and Diels-Alder cycloaddition-elimination pathways at the BH*and*HLYP/6-311++G(d,p)-LANL2DZ level of theory.[a]

Species	H	ΔH	G	ΔG
1b	–7766.871866	–	–7766.942838	–
·Sn(CH$_3$)$_3$	–6118.382302	–	–6118.426938	–
TS2	–7766.809718	–	–7766.874318	–
8	–7766.873894	–	–7766.937823	–
TS3	–7766.865396	–	–7766.927967	–
2b	–876.334420	–	–876.391465	–
HI	–6890.597830	–	–6890.621244	–
ISn(CH$_3$)$_3$	–13008.479778	–	–13008.529321	–
3b	–876.787713	–	–876.855542	–
TS1	–13885.252486	–	–13885.351528	–
Deiodination				
1b + ·Sn(CH$_3$)$_3$	–13885.254168	0.00	–13885.369776	0.00
TS1	–13885.252486	1.06	–13885.351528	11.45
3b + ISn(CH$_3$)$_3$	–13885.267491	–8.36	–13885.384863	–9.47
Diels–Alder cycloaddition and HI-elimination				
1b	–7766.871866	0.00	–7766.942838	0.00
TS2	–7766.809718	39.00	–7766.874318	43.00
8	–7766.873894	–1.27	–7766.937823	3.15
TS3	–7766.865396	4.06	–7766.927967	9.33
2b + HI	–7766.932250	–37.89	–7767.012709	–43.84

[a] 6-311++G(d,p) basis set for the C, H, O, and N atoms and 3-21G for the Sn and I atoms

Table AP3. Calculated enthalpies (H, in *a.u.*, 298.15 K), Gibbs free energies (G, in *a.u.*, 298.15 K), relative enthalpies (ΔG, in kcal/mol, 298.15 K), and relative Gibbs free energies (ΔG, in kcal/mol, 298.15 K) of reactants, products, and transition states on radical oxidation pathways by $\cdot CH_3$ at the BH*and*HLYP/6-311++G(d,p) level of theory.

Species	H	ΔH	G	ΔG
TS24–CH3	–916.606226	–17.21	–916.673559	–2.63
TS25–CH3	–916.615158	–22.81	–916.682339	–8.14
TS26–CH3	–916.602552	–14.90	–916.669677	–0.20
TS27–CH3	–916.593980	–9.52	–916.661831	4.73
TS29–CH3	–916.602850	–15.09	–916.670711	–0.85
TS28–CH3	–916.604669	–16.23	–916.671518	–1.35
3b + $\cdot CH_3$	–916.578807	0.00	–916.669361	0.00
6b + $\cdot CH_3$	–916.635407	–35.52	–916.717293	–30.08
14 + $\cdot CH_3$	–916.635801	–35.76	–916.717789	–30.39
21 + $\cdot CH_3$	–916.618724	–25.05	–916.701260	–20.02
18 + $\cdot CH_3$	–916.622193	–27.23	–916.704182	–21.85
17 + $\cdot CH_3$	–916.611887	–20.76	–916.694565	–15.82
20 + $\cdot CH_3$	–916.618778	–25.08	–916.700834	–19.75
TS10 + $\cdot CH_3$	–916.569895	5.59	–916.651589	11.15
TS11 + $\cdot CH_3$	–916.575098	2.33	–916.656673	7.96
2b + CH_4	–916.782403	–127.76	–916.860554	–119.98
2b′ + CH_4	–916.778208	–125.13	–916.856330	–117.32
23 + CH_4	–916.729160	–94.35	–916.807862	–86.91
22 + CH_4	–916.722862	–90.40	–916.801704	–83.05
$\cdot CH_3$	–39.791094	–	–39.813819	–
CH_4	–40.447983	–	–40.469089	–

Table AP4. Calculated enthalpies (H, in *a.u.*, 298.15 K), Gibbs free energies (G, in *a.u.*, 298.15 K), relative enthalpies (ΔG, in kcal/mol, 298.15 K), and relative Gibbs free energies (ΔG, in kcal/mol, 298.15 K) of reactants, products, and transition statess on radical oxidation pathways by $\cdot Sn(CH_3)_3$ at the BH*and*HLYP/6-311++G(d,p)-LANL2DZ level of theory.[a]

	H	ΔH	G	ΔG
TS24–$Sn(CH_3)_3$	–999.690015	–15.45	–999.776240	0.77
TS25–$Sn(CH_3)_3$	–999.699995	–21.71	–999.786679	–5.78
TS26–$Sn(CH_3)_3$	–999.684647	–12.08	–999.772117	3.36
TS27–$Sn(CH_3)_3$	–999.676204	–6.78	–999.763876	8.53
TS29–$Sn(CH_3)_3$	–999.686575	–13.29	–999.773040	2.78
TS28–$Sn(CH_3)_3$	–999.685788	–12.80	–999.772599	3.06
3b + $\cdot Sn(CH_3)_3$	–999.665393	0.00	–999.777474	0.00
6b + $\cdot Sn(CH_3)_3$	–999.721993	–35.52	–999.825406	–30.08
14 + $\cdot Sn(CH_3)_3$	–999.722387	–35.76	–999.825902	–30.39
21 + $\cdot Sn(CH_3)_3$	–999.705310	–25.05	–999.809373	–20.02
18 + $\cdot Sn(CH_3)_3$	–999.708779	–27.23	–999.812295	–21.85
17 + $\cdot Sn(CH_3)_3$	–999.698473	–20.76	–999.802678	–15.82
20 + $\cdot Sn(CH_3)_3$	–999.705364	–25.08	–999.808947	–19.75
TS10 + $\cdot Sn(CH_3)_3$	–999.656481	5.59	–999.759702	11.15
TS11 + $\cdot Sn(CH_3)_3$	–999.661684	2.33	–999.764786	7.96
2b + $HSn(CH_3)_3$	–999.831508	–104.24	–999.931876	–96.89
2b′ + $HSn(CH_3)_3$	–999.827313	–101.61	–999.927652	–94.24
23 + $HSn(CH_3)_3$	–999.778265	–70.83	–999.879184	–63.82
22 + $HSn(CH_3)_3$	–999.771967	–66.88	–999.873026	–59.96
$\cdot Sn(CH_3)_3$	–122.877680	–	–122.921932	–
$HSn(CH_3)_3$	–123.497088	–	–123.540411	–

[a] 6-311++G(d,p) basis set for the C, H, O, and N atoms and LANL2DZ for the Sn atom.

Table AP5. Calculated geometries of stationary points on the potential energy profile of the tandem radical cyclization at the BH*and*HLYP/6-311++G(d,p) level of theory.

Species	Geometries			
2a	Atomic			
	Number	x	y	z
	6	-2.567131	2.172385	-3.060344
	6	-1.723361	1.235220	-3.690622
	6	-1.145463	0.230852	-2.974415
	6	-1.382526	0.112055	-1.587405
	6	-2.232769	1.055971	-0.950901
	6	-2.815147	2.084169	-1.723461
	7	-0.788169	-0.900890	-0.914218
	6	-1.033423	-0.972077	0.356961
	6	-1.859194	-0.092208	1.091935
	6	-2.464336	0.929425	0.437215
	6	-0.505841	-1.974231	1.280780
	7	-1.010938	-1.684448	2.516811
	6	-1.883775	-0.512492	2.527577
	6	0.320780	-3.026157	1.087136
	6	0.637373	-3.810579	2.221576
	6	0.136237	-3.523168	3.448417
	6	-0.745510	-2.404413	3.664582
	8	-1.242267	-2.070724	4.727536
	1	-3.015244	2.959365	-3.641586
	1	-1.536873	1.317830	-4.747398
	1	-0.499122	-0.492983	-3.438368
	1	-3.459050	2.797728	-1.237361
	1	-3.105843	1.634672	0.939417
	1	-2.871948	-0.789591	2.879602
	1	-1.488316	0.237921	3.204102
	1	0.708360	-3.239457	0.109947
	1	1.293289	-4.656965	2.105296
	1	0.375207	-4.117210	4.311189
·OCH_3	Atomic			
	Number	X	Y	Z
	6	-1.285593	1.946948	-0.000116
	1	-0.887328	0.934534	-0.000038
	1	-0.920999	2.497131	0.871070
	1	-0.920623	2.497103	-0.871127
	8	-2.653250	1.998792	0.000211
3b	Atomic			
	Number	X	Y	Z
	6	-4.483783	0.287362	0.575302
	6	-4.415153	1.622459	0.936909

	6	-3.241492	2.334889	0.769348
	6	-2.135555	1.699818	0.237854
	6	-2.171551	0.361001	-0.132457
	6	-3.369976	-0.345675	0.041659
	6	-1.001181	-0.318286	-0.695668
	6	0.188624	0.199939	-0.875139
	6	1.470441	-0.243939	-1.443899
	7	2.538984	-0.325735	-0.438945
	6	3.240940	0.790281	-0.067496
	6	4.203191	0.755962	0.881176
	6	4.482216	-0.483211	1.510006
	6	3.799167	-1.589839	1.162712
	6	2.760593	-1.566726	0.157529
	8	2.111777	-2.537743	-0.172899
	6	2.940149	2.025464	-0.721565
	7	2.730179	3.027072	-1.225696
	8	-3.361617	-1.642078	-0.335022
	6	-4.526863	-2.415527	-0.173801
	1	-5.403489	-0.249533	0.711294
	1	-5.286787	2.101137	1.349156
	1	-3.187765	3.372598	1.047723
	1	-1.217650	2.245595	0.100327
	1	-1.144822	-1.353274	-0.982688
	1	1.798206	0.420782	-2.234958
	1	1.363075	-1.240234	-1.860449
	1	4.732787	1.652657	1.137861
	1	5.245526	-0.529152	2.267102
	1	3.983066	-2.544359	1.620061
	1	-4.279942	-3.405087	-0.531300
	1	-4.819470	-2.473676	0.870963
	1	-5.349587	-2.016355	-0.760723
4b′	Atomic Number	X	Y	Z
	6	4.582660	-0.160267	0.000269
	6	4.638447	-1.544272	0.000065
	6	3.477134	-2.291708	-0.000232
	6	2.253666	-1.649104	-0.000318
	6	2.153746	-0.259456	-0.000109
	6	3.356702	0.484089	0.000185
	6	0.909491	0.491371	-0.000236
	6	-0.390228	0.162434	-0.000149
	6	-1.443572	1.251514	-0.000382
	7	-2.703211	0.527977	-0.000026
	6	-2.553340	-0.821672	0.000311

	6	-3.615871	-1.655432	0.000640
	6	-4.898995	-1.056671	0.000617
	6	-5.052596	0.289044	0.000279
	6	-3.921394	1.182131	-0.000070
	8	-3.964675	2.399712	-0.000446
	6	-1.102370	-1.130198	0.000251
	7	-0.672928	-2.306759	0.000371
	8	3.237556	1.826014	0.000368
	6	4.396295	2.629089	0.000798
	1	5.495375	0.404319	0.000490
	1	5.598410	-2.031466	0.000135
	1	3.517810	-3.366352	-0.000400
	1	1.360102	-2.242807	-0.000566
	1	1.079572	1.555250	-0.000420
	1	-1.388443	1.887247	-0.877559
	1	-1.388256	1.887812	0.876372
	1	-3.479732	-2.719330	0.000903
	1	-5.770211	-1.689577	0.000874
	1	-6.023455	0.749299	0.000254
	1	4.048090	3.651965	0.000978
	1	4.996056	2.452763	-0.887269
	1	4.995695	2.452325	0.889021
4b	Atomic Number	X	Y	Z
	6	3.989604	-1.181134	1.223112
	6	4.142570	-2.070305	0.174134
	6	3.329480	-1.990162	-0.941739
	6	2.348847	-1.018187	-0.987339
	6	2.141571	-0.138642	0.070083
	6	3.001471	-0.206064	1.175044
	6	1.068231	0.852872	-0.050196
	6	0.101102	1.156763	0.811759
	6	-0.949625	2.207190	0.544440
	7	-1.882050	2.053159	1.651563
	6	-1.511393	1.104877	2.553100
	6	-2.255682	0.838007	3.648163
	6	-3.443031	1.590902	3.816142
	6	-3.814752	2.536651	2.920652
	6	-3.022519	2.828045	1.752428
	8	-3.275921	3.660878	0.899746
	6	-0.235889	0.504375	2.095915
	7	0.360068	-0.405656	2.711677
	8	2.839091	0.730722	2.123748
	6	3.563922	0.627052	3.327266

	1	4.646379	-1.247121	2.069738
	1	4.912655	-2.820386	0.230153
	1	3.456356	-2.672294	-1.763434
	1	1.709197	-0.944113	-1.851070
	1	1.037729	1.371018	-0.998812
	1	-1.467300	2.059850	-0.396586
	1	-0.545139	3.213980	0.549279
	1	-1.949954	0.086204	4.349478
	1	-4.062260	1.403822	4.677068
	1	-4.714435	3.111170	3.042545
	1	3.218355	1.437041	3.953573
	1	4.631265	0.737943	3.156426
	1	3.365296	-0.319615	3.820375
5b	Atomic			
	Number	X	Y	Z
	6	1.691533	-0.520055	-0.116726
	7	0.661072	-0.384649	0.949395
	6	-0.438465	-0.277735	0.331408
	6	-0.366761	-0.296453	-1.123118
	6	0.914080	-0.424121	-1.431665
	6	-1.840107	-0.136168	0.713019
	7	-2.552465	-0.072077	-0.460610
	6	-1.738360	-0.160969	-1.689066
	6	-2.451203	-0.068351	1.913643
	6	-3.861634	0.073026	1.916299
	6	-4.564980	0.137411	0.761995
	6	-3.922822	0.066153	-0.529166
	6	2.327587	-1.879204	0.009137
	6	3.653519	-2.054332	0.211758
	6	4.527615	-0.956294	0.319222
	6	4.026469	0.358369	0.218417
	6	2.704940	0.590264	0.014822
	8	-4.485604	0.116983	-1.609477
	8	2.132352	1.796096	-0.102726
	6	2.929623	2.947836	0.052506
	1	1.390532	-0.477536	-2.392291
	1	-2.060982	-1.011805	-2.277836
	1	-1.881731	0.733137	-2.284580
	1	-1.876950	-0.120469	2.818435
	1	-4.380600	0.130088	2.858073
	1	-5.634161	0.244312	0.754470
	1	1.654275	-2.716054	-0.057534
	1	4.046784	-3.053237	0.298493
	1	5.578322	-1.112281	0.482952

	1	4.710967	1.182185	0.305919
	1	2.263800	3.791587	-0.058029
	1	3.387532	2.972642	1.037076
	1	3.701941	2.993210	-0.710374
6b	Atomic			
	Number	X	Y	Z
	6	4.148293	0.669153	-0.228574
	6	3.667686	2.021824	-0.267604
	6	2.402599	2.331789	0.034775
	6	1.464668	1.284263	0.532876
	6	1.909942	-0.127077	0.231873
	6	3.285911	-0.370097	-0.005577
	7	0.080921	1.604047	0.222138
	6	-0.715469	0.605389	0.196559
	6	-0.365743	-0.780985	0.298867
	6	0.956453	-1.141291	0.246268
		-2.169165	0.672599	0.000529
	7	-2.645494	-0.606750	0.033151
	6	-1.603729	-1.613723	0.233785
	6	-2.994829	1.726923	-0.175662
	6	-4.373988	1.445771	-0.327670
	6	-4.847557	0.176351	-0.292756
	6	-3.974481	-0.954019	-0.099631
	8	-4.312723	-2.125175	-0.050359
	8	3.633385	-1.673232	-0.050295
	6	4.958266	-2.015679	-0.385273
	1	5.182948	0.486129	-0.447641
	1	4.356857	2.792662	-0.567672
	1	2.033106	3.341217	0.000012
	1	1.512599	1.365513	1.637842
	1	1.263013	-2.167628	0.150486
	1	-1.802023	-2.170048	1.145143
	1	-1.607971	-2.320627	-0.589828
	1	-2.602241	2.724996	-0.195837
	1	-5.061267	2.262159	-0.473383
	1	-5.893376	-0.042395	-0.406498
	1	4.999320	-3.095532	-0.378519
	1	5.219173	-1.650086	-1.374570
	1	5.661757	-1.625182	0.344766
7b	Atomic			
	Number	X	Y	Z
	6	0.167260	-0.200303	-0.929928
	6	-0.191896	1.198568	-0.805515
	6	1.634385	-0.262649	-0.928797

	7	2.102477	1.007698	-0.746969
	6	1.046521	2.011923	-0.619142
	6	2.474515	-1.311249	-1.058983
	6	3.862280	-1.035627	-1.001473
	6	4.327130	0.223739	-0.818374
	6	3.437322	1.348742	-0.671833
	8	3.768090	2.509840	-0.498382
	6	-1.473795	1.563701	-1.044471
	6	-2.413769	0.539026	-1.291097
	6	-2.029421	-0.873876	-0.894732
	7	-0.618685	-1.187492	-1.058788
	6	-3.649918	0.782242	-1.880870
	6	-4.441750	-0.253188	-2.329272
	6	-4.000816	-1.608052	-2.219609
	6	-2.853603	-1.910738	-1.591903
	1	1.105609	2.483690	0.357148
	1	1.176196	2.785314	-1.368552
	1	2.086436	-2.301863	-1.195697
	1	4.561942	-1.847859	-1.104381
	1	5.378796	0.438944	-0.771674
	1	-1.765988	2.596856	-1.141238
	1	-3.957387	1.802363	-2.043938
	1	-5.376961	-0.039761	-2.816376
	1	-4.596882	-2.386779	-2.664174
	1	-2.497589	-2.921984	-1.500934
	8	-2.196905	-1.023731	0.529897
	6	-3.470498	-0.781005	1.081950
	1	-4.240644	-1.385640	0.611537
	1	-3.746665	0.267791	1.012517
	1	-3.396789	-1.056642	2.126053
9	Atomic Number	X	Y	Z
	6	2.680100	-1.013675	0.629924
	6	2.981956	-2.295130	1.048106
	6	1.968229	-3.191296	1.344816
	6	0.643137	-2.803257	1.225236
	6	0.312163	-1.499643	0.805080
	6	1.357668	-0.627803	0.509371
	6	-1.101657	-1.156726	0.695169
	6	-1.694737	0.022529	0.497175
	6	-3.189844	0.171956	0.519444
	7	-3.663090	1.119230	-0.498595
	6	-2.885761	2.206547	-0.812854
	6	-3.315642	3.165548	-1.662767

	6	-4.601670	3.023651	-2.239452
	6	-5.375316	1.961717	-1.934316
	6	-4.946618	0.945076	-1.000855
	8	-5.629369	0.000530	-0.651367
	6	-1.559358	2.181117	-0.226562
	7	-1.000316	1.232975	0.317454
	1	3.465544	-0.317667	0.393402
	1	4.007144	-2.609450	1.143664
	1	2.219279	-4.183846	1.667472
	8	-0.391122	-3.625563	1.502119
	1	1.122967	0.365350	0.179932
	1	-1.768930	-1.992812	0.803684
	1	-3.686071	-0.769614	0.346219
	1	-3.510093	0.543420	1.492290
	1	-2.675653	3.995137	-1.893541
	1	-4.958825	3.771733	-2.926181
	1	-6.356933	1.830677	-2.350963
	6	-0.134261	-4.947877	1.912751
	1	-1.101338	-5.406175	2.063543
	1	0.422696	-4.969180	2.845289
	1	0.409822	-5.498582	1.150512
10	Atomic Number	X	Y	Z
	6	1.855829	0.368321	-0.746586
	7	1.119649	1.597855	-0.680054
	6	-0.134553	1.249477	-0.520980
	6	-0.386704	-0.112675	-0.488175
	6	0.878529	-0.815943	-0.588572
	6	-1.389737	1.969827	-0.365218
	7	-2.360675	1.001959	-0.261637
	6	-1.837805	-0.369954	-0.317280
	6	-1.704620	3.282422	-0.329294
	6	-3.074544	3.613926	-0.183912
	6	-4.031360	2.660180	-0.084674
	6	-3.708847	1.255399	-0.120247
	6	3.023829	0.327700	-1.623153
	6	3.987581	-0.583082	-1.463985
	6	3.995002	-1.459778	-0.315895
	6	3.060967	-1.380063	0.639186
	6	1.892943	-0.505398	0.530058
	8	-4.502492	0.332556	-0.035517
	8	1.436706	0.046192	1.700842
	6	0.754073	-0.838332	2.563593

	1	0.998567	-1.743844	-1.118141
	1	-2.092848	-0.900797	0.595514
	1	-2.293932	-0.909100	-1.143157
	1	-0.938852	4.029539	-0.408184
	1	-3.358788	4.652242	-0.151223
	1	-5.070617	2.908381	0.027778
	1	3.074156	1.075362	-2.395394
	1	4.821123	-0.614550	-2.143617
	1	4.830309	-2.126298	-0.184907
	1	3.170443	-1.935686	1.554813
	1	0.343575	-0.237143	3.363238
	1	-0.053065	-1.347661	2.043354
	1	1.425160	-1.580032	2.988427
11	Atomic			
	Number	X	Y	Z
	6	1.653806	-1.429215	-0.877132
	6	2.950856	-2.087860	-0.996272
	6	1.640893	-0.043370	-0.227880
	6	4.057386	-1.525763	-0.496840
	6	2.941768	0.521242	0.169575
	6	4.067225	-0.208403	0.098081
	6	-0.389083	-0.876922	0.467158
	6	1.017925	-1.223605	0.515092
	6	-1.721616	-1.398426	0.855563
	6	-0.515621	0.296398	-0.257637
	6	-1.928428	0.623218	-0.388417
	7	0.604799	0.845121	-0.677403
	7	-2.601949	-0.372497	0.278921
	6	-2.590981	1.641328	-0.978780
	6	-3.972698	-0.433579	0.419286
	6	-4.667416	0.658816	-0.215323
	6	-4.004099	1.637767	-0.876048
	8	-4.488253	-1.353847	1.032307
	8	2.837150	1.775072	0.617359
	6	4.016316	2.462228	0.971715
	1	0.944431	-1.588617	-1.672185
	1	2.998715	-3.017855	-1.536020
	1	5.001003	-2.036971	-0.586403
	1	5.004147	0.190565	0.437437
	1	1.494669	-1.702126	1.350664
	1	-1.954544	-2.371250	0.430843
	1	-1.880893	-1.465053	1.928152
	1	-2.055034	2.413226	-1.496271
	1	-5.738904	0.652030	-0.136817

	1	-4.562142	2.435690	-1.336417
	1	3.709575	3.459696	1.251006
	1	4.507174	1.983180	1.814381
	1	4.701798	2.511228	0.130630
12	Atomic			
	Number	X	Y	Z
	6	-0.805022	0.950436	1.913842
	7	-1.503665	-0.198698	1.251884
	6	-1.333069	0.080583	-0.102789
	6	-0.685346	1.289829	-0.352506
	6	-0.337234	1.855309	0.834358
	6	-1.645578	-0.577477	-1.310470
	7	-1.195096	0.251714	-2.326761
	6	-0.557450	1.477173	-1.827848
	6	-2.258269	-1.763123	-1.608011
	6	-2.407464	-2.092449	-2.969547
	6	-1.963892	-1.271694	-3.959050
	6	-1.314961	-0.013905	-3.667529
	6	-1.352836	1.484832	3.165179
	6	-1.505677	0.715969	4.246395
	6	-1.021475	-0.646678	4.281846
	6	-0.388181	-1.197560	3.242778
	6	-0.255515	-0.497018	1.963852
	8	-0.891207	0.776337	-4.496884
	8	0.787246	-0.879094	1.171912
	6	2.067601	-0.508887	1.646948
	1	0.162903	2.786623	1.018185
	1	0.469361	1.527211	-2.172997
	1	-1.080670	2.348953	-2.205187
	1	-2.610540	-2.403200	-0.822327
	1	-2.887272	-3.020665	-3.231173
	1	-2.076392	-1.521574	-4.997740
	1	-1.605407	2.531437	3.190470
	1	-1.930127	1.130363	5.144576
	1	-1.115920	-1.198006	5.201788
	1	0.076481	-2.166711	3.314543
	1	2.781229	-0.872393	0.920606
	1	2.147000	0.571936	1.726633
	1	2.277442	-0.958573	2.613024
13	Atomic			
	Number	X	Y	Z
	6	1.682561	-0.145648	0.419565
	7	0.748501	0.815774	-0.220389
	6	-0.490110	0.207640	-0.032587

	6	-0.415201	-1.042405	0.586053
	6	0.885369	-1.318703	0.873932
	6	-1.830807	0.544918	-0.316395
	7	-2.597862	-0.519803	0.133800
	6	-1.794640	-1.595745	0.731044
	6	-2.428149	1.627911	-0.899889
	6	-3.831696	1.607981	-1.020458
	6	-4.575209	0.559814	-0.575995
	6	-3.965567	-0.594087	0.044236
	6	3.012634	-0.314495	-0.200370
	6	3.878330	0.706505	-0.279874
	6	3.584840	1.977546	0.345292
	6	2.455578	2.210388	1.021072
	6	1.405169	1.199054	1.065102
	8	-4.563008	-1.570885	0.468814
	8	3.215426	-1.566922	-0.629719
	6	4.468943	-1.889831	-1.190588
	1	1.309699	-2.191662	1.327774
	1	-2.097684	-1.757221	1.759613
	1	-1.950455	-2.521166	0.187398
	1	-1.834771	2.448901	-1.253575
	1	-4.326886	2.447718	-1.478612
	1	-5.645440	0.543327	-0.666759
	1	4.831768	0.584989	-0.758270
	1	4.348540	2.735759	0.304819
	1	2.313792	3.121756	1.575371
	1	0.740613	1.198847	1.913415
	1	4.428154	-2.941840	-1.432870
	1	4.646984	-1.315119	-2.094742
	1	5.269009	-1.707215	-0.478765
14	Atomic			
	Number	X	Y	Z
	6	4.055065	-1.560427	-0.361909
	6	4.126869	-0.125081	-0.241928
	6	3.023311	0.619218	0.026189
	6	1.744298	-0.027883	0.204578
	6	1.751651	-1.518041	0.483812
	6	2.944251	-2.234002	-0.066008
	7	0.654133	0.687672	0.163294
	6	-0.507673	0.034154	0.168040
	6	-0.650661	-1.383695	0.090949
	6	0.433134	-2.165438	0.173461
	6	-1.807272	0.632820	0.090576
	7	-2.723775	-0.381956	-0.044166

	6	-2.104893	-1.706175	-0.092322
	6	-2.208942	1.933558	0.130439
	6	-3.593551	2.185149	0.033137
	6	-4.494951	1.176734	-0.095895
	6	-4.083815	-0.205895	-0.145428
	8	-4.825761	-1.168010	-0.266685
	8	2.990814	1.956948	0.077398
	6	4.174239	2.671720	-0.186429
	1	4.932822	-2.080601	-0.705498
	1	5.070647	0.351080	-0.429554
	1	1.872055	-1.582961	1.583289
	1	2.896628	-3.306924	-0.142992
	1	0.390320	-3.239118	0.100985
	1	-2.507871	-2.332450	0.695583
	1	-2.323118	-2.182421	-1.042504
	1	-1.484789	2.718212	0.233925
	1	-3.942744	3.203678	0.062961
	1	-5.550219	1.363639	-0.170114
	1	3.917288	3.717638	-0.099488
	1	4.537743	2.470468	-1.190805
	1	4.950000	2.429969	0.535574
15	Atomic			
	Number	X	Y	Z
	6	0.018669	-0.324358	-0.250873
	6	-0.292131	1.079360	-0.298442
	6	1.451271	-0.466956	-0.201603
	7	1.996638	0.790008	-0.254968
	6	0.993437	1.850345	-0.358063
	6	2.239698	-1.570862	-0.120021
	6	3.636770	-1.366257	-0.088423
	6	4.172104	-0.120282	-0.139902
	6	3.345710	1.060947	-0.234044
	8	3.748912	2.210221	-0.294438
	6	-1.563600	1.473370	-0.258805
	6	-2.614473	0.428387	-0.009753
	6	-2.133912	-0.947023	-0.447744
	7	-0.850548	-1.298426	-0.374444
	6	-3.937218	0.789655	-0.615512
	6	-4.734684	-0.122454	-1.183044
	6	-4.320262	-1.492630	-1.305248
	6	-3.062604	-1.880743	-0.944285
	8	-2.738901	0.460370	1.434991
	6	-3.603117	-0.470142	2.050013
	1	1.110742	2.550353	0.460896

	1	1.126174	2.394266	-1.287329
	1	1.797845	-2.547620	-0.081437
	1	4.289694	-2.220066	-0.021734
	1	5.233861	0.042437	-0.116481
	1	-1.868391	2.505743	-0.281563
	1	-4.248654	1.815191	-0.505485
	1	-5.701021	0.162684	-1.562859
	1	-5.001322	-2.208597	-1.731104
	1	-2.721031	-2.888767	-1.103551
	1	-4.611218	-0.416680	1.648890
	1	-3.627148	-0.203897	3.098922
	1	-3.231290	-1.486579	1.952443
16	Atomic			
	Number	X	Y	Z
	6	-1.639067	-0.440352	0.000239
	7	-0.747800	0.628327	-0.000127
	6	0.510113	0.090423	0.000243
	6	0.434448	-1.268499	0.000848
	6	-0.921639	-1.619223	0.000797
	6	1.884566	0.527319	-0.000323
	7	2.621969	-0.638166	0.000397
	6	1.800137	-1.852654	0.001078
	6	2.517799	1.730300	-0.001496
	6	3.931575	1.725589	-0.001782
	6	4.649310	0.576480	-0.000954
	6	4.000457	-0.707740	0.000159
	6	-3.084775	-0.355100	-0.000305
	6	-3.865998	0.765186	0.000236
	6	-3.477347	2.114358	0.001282
	6	-2.175645	2.642666	0.001557
	6	-0.982581	2.005579	0.000858
	8	4.556136	-1.794233	0.000738
	8	-3.604618	-1.605250	-0.001346
	6	-4.999019	-1.791855	-0.000578
	1	-1.362984	-2.592998	0.000980
	1	2.029061	-2.450487	-0.875099
	1	2.029103	-2.449606	0.877843
	1	1.976134	2.654282	-0.002348
	1	4.449272	2.670268	-0.002700
	1	5.723482	0.574651	-0.001188
	1	-4.928496	0.604400	-0.000163
	1	-4.278404	2.832184	0.001879
	1	-2.099776	3.717014	0.002411
	1	-0.080100	2.580535	0.001264

	1	-5.152865	-2.861645	-0.001034
	1	-5.454910	-1.364006	0.888049
	1	-5.456034	-1.363145	-0.888214
17	Atomic			
	Number	X	Y	Z
	6	-1.551700	0.279887	0.123093
	7	-0.608658	1.166980	-0.070291
	6	0.574304	0.465191	0.029592
	6	0.439738	-0.840752	0.291295
	6	-1.015430	-1.126484	0.411310
	6	1.975347	0.810594	-0.090932
	7	2.654107	-0.367754	0.116386
	6	1.764216	-1.504931	0.377513
	6	2.638909	1.962110	-0.343476
	6	4.052444	1.894302	-0.384245
	6	4.719835	0.731701	-0.181408
	6	4.025779	-0.501747	0.088624
	6	-2.931142	0.609309	0.168396
	6	-3.972250	-0.330394	0.190755
	6	-3.946726	-1.661773	-0.157021
	6	-2.857752	-2.439973	-0.662454
	6	-1.551017	-2.202148	-0.487607
	8	4.541333	-1.591359	0.282945
	8	-3.170274	1.927715	0.228150
	6	-4.476665	2.428777	0.047838
	1	-1.273299	-1.374258	1.446160
	1	1.929711	-2.281700	-0.364272
	1	1.986561	-1.933505	1.351048
	1	2.103480	2.877780	-0.503334
	1	4.610781	2.793951	-0.582399
	1	5.792514	0.680114	-0.212040
	1	-4.946976	0.056578	0.429190
	1	-4.902562	-2.159140	-0.143035
	1	-3.133779	-3.308869	-1.238636
	1	-0.832416	-2.846102	-0.965575
	1	-4.370783	3.501587	-0.027083
	1	-4.922396	2.042433	-0.863778
	1	-5.113351	2.194595	0.895996
18	Atomic			
	Number	X	Y	Z
	6	-1.776281	1.305552	1.031836
	7	-0.587919	1.889475	0.999986
	6	0.319359	0.866493	0.894974
	6	-0.206159	-0.369881	0.866504

	6	-1.681467	-0.225843	1.004465
	6	1.764260	0.794987	0.819320
	7	2.055745	-0.546573	0.748969
	6	0.858738	-1.397277	0.770726
	6	2.746169	1.725531	0.809824
	6	4.078235	1.253748	0.723721
	6	4.364574	-0.069375	0.652756
	6	3.327657	-1.070405	0.661550
	6	-2.962057	2.020681	1.184841
	6	-4.253637	1.494684	1.085717
	6	-4.642864	0.310149	0.505168
	6	-3.859099	-0.672132	-0.173460
	6	-2.534583	-0.889273	-0.039287
	8	3.494083	-2.278349	0.601675
	8	-1.835327	-1.784014	-0.746026
	6	-2.469283	-2.504810	-1.783535
	1	-2.006391	-0.593032	1.982494
	1	0.807995	-1.996675	-0.131882
	1	0.902072	-2.078029	1.616631
	1	2.510023	2.770463	0.865575
	1	4.884130	1.968433	0.714532
	1	5.374921	-0.428856	0.587748
	1	-2.852187	3.069014	1.405764
	1	-5.051647	2.138869	1.417030
	1	-5.706720	0.144764	0.453736
	1	-4.406540	-1.304530	-0.849339
	1	-1.697437	-3.105681	-2.241728
	1	-2.893786	-1.827686	-2.517938
	1	-3.245576	-3.151422	-1.386348
19	Atomic Number	X	Y	Z
	6	-1.840513	-1.031832	-0.467222
	7	-1.175645	0.200531	-0.559092
	6	0.182360	-0.064475	-0.490596
	6	0.358966	-1.409605	-0.337272
	6	-0.891950	-2.026390	-0.313368
	6	1.466334	0.585122	-0.648941
	7	2.397429	-0.429577	-0.519986
	6	1.801680	-1.747200	-0.314217
	6	1.897697	1.848034	-0.915678
	6	3.288305	2.060150	-1.036362
	6	4.192003	1.060450	-0.890387
	6	3.765389	-0.284243	-0.620188
	6	-3.231591	-1.278101	-0.608363

	6	-4.244655	-0.398457	-0.931999
	6	-4.164591	0.976135	-1.033384
	6	-3.045118	1.801189	-0.730192
	6	-1.761546	1.473731	-0.479151
	8	4.491892	-1.258226	-0.490021
	8	-0.829219	2.352996	-0.101264
	6	-1.171948	3.707505	0.101262
	1	-1.120660	-3.070177	-0.234673
	1	2.112768	-2.418845	-1.107735
	1	2.140314	-2.169188	0.626791
	1	1.202336	2.649177	-1.032375
	1	3.637270	3.056778	-1.250857
	1	5.249533	1.225040	-0.981510
	1	-3.486870	-2.319482	-0.517900
	1	-5.213626	-0.837170	-1.105605
	1	-5.067110	1.502963	-1.289972
	1	-3.266223	2.848854	-0.653105
	1	-1.514898	4.166326	-0.820783
	1	-0.264233	4.191123	0.432130
	1	-1.933879	3.800865	0.868014
20	Atomic			
	Number	X	Y	Z
	6	1.611282	0.193370	-0.813974
	7	0.483904	1.119975	-0.894023
	6	-0.526464	0.436663	-0.491052
	6	-0.273184	-0.904000	-0.093749
	6	1.073627	-1.125347	-0.256603
	6	-1.952858	0.701370	-0.337303
	7	-2.504086	-0.464362	0.138342
	6	-1.537081	-1.559487	0.332995
	6	-2.709718	1.794334	-0.568326
	6	-4.097393	1.689308	-0.299674
	6	-4.641444	0.541861	0.169128
	6	-3.842821	-0.633793	0.420322
	6	2.781581	0.733793	-0.028587
	6	3.903530	0.014056	0.194884
	6	4.118677	-1.369641	-0.084706
	6	3.205764	-2.389742	-0.200213
	6	1.811291	-2.294307	-0.112117
	8	-4.255631	-1.701961	0.839893
	1	1.957829	0.019020	-1.835021
	1	-1.545886	-1.875014	1.371338
	1	-1.824559	-2.412416	-0.273797
	1	-2.262455	2.696137	-0.939443

	1	-4.729843	2.543488	-0.473180
	1	-5.692315	0.454747	0.375333
	8	2.614819	2.000905	0.342394
	1	4.748151	0.525271	0.620858
	1	5.154578	-1.668527	-0.085771
	1	3.612678	-3.385543	-0.266781
	1	1.262619	-3.204596	0.068676
	6	3.608511	2.636277	1.116854
	1	3.215993	3.613983	1.355763
	1	4.531102	2.744610	0.554196
	1	3.799947	2.082362	2.031069
21	Atomic			
	Number	X	Y	Z
	6	-1.802077	1.047580	1.507126
	7	-0.493780	1.634917	1.803126
	6	0.350157	0.848609	1.248360
	6	-0.192200	-0.254539	0.518541
	6	-1.545152	-0.150151	0.601474
	6	1.804742	0.797107	1.140512
	7	2.089089	-0.304013	0.369700
	6	0.903766	-1.056932	-0.083104
	6	2.783850	1.584754	1.632951
	6	4.119497	1.228333	1.321041
	6	4.401509	0.144221	0.560987
	6	3.363185	-0.705469	0.028746
	6	-2.759066	2.064347	0.971659
	6	-3.964672	1.776438	0.456660
	6	-4.527199	0.487333	0.198840
	6	-3.897618	-0.727104	0.018389
	6	-2.529449	-1.006579	0.070248
	8	3.535338	-1.694906	-0.663243
	8	-2.011589	-2.164441	-0.397116
	6	-2.816135	-3.064814	-1.127451
	1	-2.193691	0.672415	2.458597
	1	0.882897	-1.093057	-1.166673
	1	0.954448	-2.076618	0.281122
	1	2.542790	2.440658	2.233293
	1	4.925050	1.835299	1.698428
	1	5.411547	-0.132568	0.320527
	1	-2.460127	3.091937	1.085846
	1	-4.604204	2.610462	0.214204
	1	-5.591318	0.479535	0.029280
	1	-4.541179	-1.535611	-0.279278
	1	-2.146445	-3.831650	-1.489931

	1	-3.292569	-2.571001	-1.969065
	1	-3.570796	-3.522995	-0.495095
TS4	Atomic			
	Number	X	Y	Z
	6	-4.428512	-0.150545	0.394155
	6	-4.538467	-1.474186	-0.004381
	6	-3.481036	-2.113296	-0.621404
	6	-2.303210	-1.420752	-0.838968
	6	-2.158521	-0.098515	-0.441269
	6	-3.246446	0.538611	0.177017
	6	-0.932548	0.661992	-0.677300
	6	0.294053	0.220502	-0.832391
	6	1.562451	0.873335	-1.176621
	7	2.637331	0.341195	-0.339458
	6	2.463566	-0.849435	0.298263
	6	3.432231	-1.388087	1.074327
	6	4.648067	-0.675558	1.210904
	6	4.835966	0.497523	0.571450
	6	3.818689	1.068873	-0.275636
	8	3.929622	2.104835	-0.903775
	6	1.211211	-1.545435	0.106609
	7	0.513985	-2.468019	0.187292
	8	-3.054847	1.825300	0.537879
	6	-4.111800	2.536783	1.138230
	1	-5.262418	0.328535	0.871309
	1	-5.462390	-1.998866	0.169025
	1	-3.570069	-3.137634	-0.936923
	1	-1.481321	-1.904981	-1.332211
	1	-1.058706	1.738264	-0.726660
	1	1.506829	1.945413	-1.012106
	1	1.825555	0.719529	-2.220324
	1	3.266087	-2.327458	1.563770
	1	5.426900	-1.082958	1.832160
	1	5.749994	1.055789	0.654972
	1	-3.736598	3.534344	1.317458
	1	-4.401120	2.086991	2.083849
	1	-4.974915	2.589366	0.480454
TS5	Atomic			
	Number	X	Y	Z
	6	-0.042884	-0.164777	-0.066322
	6	-0.042047	-0.087536	1.313568
	6	1.152636	-0.027593	2.012142
	6	2.357467	-0.042503	1.325456
	6	2.375100	-0.115077	-0.076893

	6	1.160075	-0.179586	-0.748463
	6	3.667707	-0.142635	-0.765683
	6	3.943103	0.014820	-2.039849
	6	5.211313	-0.088572	-2.783894
	7	5.574371	1.124203	-3.546569
	6	4.640301	1.782870	-4.306947
	6	4.953341	2.849281	-5.073261
	6	6.296565	3.299690	-5.077203
	6	7.229030	2.662323	-4.342978
	6	6.916345	1.499334	-3.543646
	8	7.739864	0.870828	-2.907601
	6	3.303945	1.279819	-4.168558
	7	2.601176	0.609017	-3.516223
	1	-0.970163	-0.216839	-0.609290
	1	-0.970683	-0.076048	1.858115
	1	1.135475	0.031333	3.083904
	1	1.168377	-0.242115	-1.820037
	1	4.521082	-0.317646	-0.120978
	1	6.033772	-0.266976	-2.102324
	1	5.174890	-0.922400	-3.481830
	1	4.187657	3.335216	-5.646159
	1	6.566023	4.155337	-5.671735
	1	8.256943	2.974461	-4.327356
	8	3.559680	0.015298	1.938490
	6	3.616494	0.072757	3.344069
	1	4.666303	0.101294	3.599436
	1	3.130998	0.968429	3.721586
	1	3.160796	-0.805248	3.793553
TS6	Atomic			
	Number	X	Y	Z
	6	4.082033	-0.476601	0.475457
	6	3.880260	-1.825735	0.125986
	6	2.779566	-2.224678	-0.568356
	6	1.782510	-1.271301	-0.920565
	6	1.980451	0.094409	-0.565046
	6	3.144956	0.473838	0.124939
	7	0.061360	-1.786089	-0.118481
	6	-0.683909	-0.773835	-0.238475
	6	-0.363173	0.565123	-0.743102
	6	0.903771	1.013231	-0.786613
	6	-2.103692	-0.723159	0.174954
	7	-2.605382	0.491004	-0.188923
	6	-1.630233	1.357299	-0.847071
	6	-2.872544	-1.650109	0.785920

	6	-4.222136	-1.303202	1.035758
	6	-4.724140	-0.099123	0.669785
	6	-3.913325	0.890454	0.006508
	8	-4.282701	1.990562	-0.368410
	8	3.243634	1.784651	0.424019
	6	4.393627	2.249495	1.093442
	1	4.963493	-0.204564	1.024033
	1	4.632945	-2.544991	0.400335
	1	2.652443	-3.249938	-0.866039
	1	1.243355	-1.448547	-1.836971
	1	1.111418	2.066317	-0.872227
	1	-1.939758	1.538083	-1.872326
	1	-1.581339	2.314917	-0.341686
	1	-2.461406	-2.601846	1.061297
	1	-4.862747	-2.016142	1.526962
	1	-5.748177	0.168614	0.854479
	1	4.263441	3.316374	1.205261
	1	4.486630	1.793953	2.075247
	1	5.291498	2.054544	0.513789
TS7	Atomic			
	Number	X	Y	Z
	6	1.868338	-0.270157	-0.643887
	7	0.615932	-0.890633	0.694837
	6	-0.432114	-0.448956	0.164761
	6	-0.379474	0.289974	-1.100801
	6	0.864114	0.409184	-1.523412
	6	-1.846503	-0.500918	0.568410
	7	-2.563255	0.156175	-0.396954
	6	-1.756839	0.699928	-1.501464
	6	-2.449686	-1.051414	1.642359
	6	-3.857748	-0.921725	1.731400
	6	-4.568237	-0.274022	0.778291
	6	-3.933850	0.317269	-0.374517
	6	2.436158	-1.500002	-1.123779
	6	3.628108	-1.969246	-0.643755
	6	4.373550	-1.198578	0.248507
	6	3.937174	0.073496	0.624901
	6	2.743644	0.560911	0.153615
	8	-4.499181	0.913848	-1.275342
	8	2.252944	1.781323	0.417995
	6	2.974647	2.636669	1.275436
	1	1.188414	0.924451	-2.410369
	1	-2.087656	0.269384	-2.439652
	1	-1.893174	1.773815	-1.557998

	1	-1.870441	-1.562191	2.387135
	1	-4.370734	-1.349138	2.576335
	1	-5.636185	-0.171846	0.837824
	1	1.860246	-2.075720	-1.827327
	1	4.001335	-2.924126	-0.970780
	1	5.311611	-1.565610	0.626057
	1	4.555234	0.670326	1.269338
	1	2.395830	3.546200	1.347552
	1	3.082491	2.196444	2.262406
	1	3.955359	2.864090	0.867100
TS8	Atomic Number	X	Y	Z
	6	0.316747	-0.170420	-0.071218
	6	0.186833	1.262858	0.229585
	6	1.767786	-0.430228	-0.195642
	7	2.429802	0.718387	0.123565
	6	1.550017	1.828262	0.481816
	6	2.432049	-1.554946	-0.537837
	6	3.846027	-1.488053	-0.552357
	6	4.505671	-0.349021	-0.230955
	6	3.804558	0.852588	0.143891
	8	4.313411	1.915902	0.457245
	6	-0.975725	1.899309	0.057692
	6	-2.147050	1.127539	-0.289316
	6	-2.304504	-0.181624	0.279709
	7	-0.583132	-1.037059	-0.218696
	6	-2.998913	1.537342	-1.310843
	6	-3.970106	0.694820	-1.812891
	6	-4.115442	-0.598935	-1.285606
	6	-3.331664	-1.017197	-0.251317
	1	1.711493	2.098078	1.521177
	1	1.778557	2.695501	-0.126753
	1	1.895114	-2.450684	-0.782738
	1	4.407762	-2.365757	-0.824431
	1	5.578587	-0.293219	-0.237683
	1	-1.023740	2.976767	0.048678
	1	-2.863266	2.517088	-1.737977
	1	-4.606741	1.024040	-2.614954
	1	-4.871831	-1.253552	-1.683311
	1	-3.463580	-1.985915	0.197952
	8	-1.990607	-0.367348	1.610176
	6	-2.947001	0.164209	2.506911
	1	-3.927757	-0.275002	2.343527
	1	-3.017047	1.244739	2.407373

	1	-2.602179	-0.083972	3.501683
TS9	Atomic			
	Number	X	Y	Z
	6	0.189960	-0.195271	-0.999666
	6	-0.177012	1.187301	-0.883209
	6	1.651229	-0.266156	-0.927619
	7	2.112678	1.006038	-0.738334
	6	1.051957	2.009697	-0.668759
	6	2.495235	-1.317069	-1.008625
	6	3.878997	-1.041048	-0.890830
	6	4.336999	0.220123	-0.701389
	6	3.443152	1.347504	-0.608858
	8	3.766384	2.510754	-0.435904
	6	-1.468077	1.538662	-1.084779
	6	-2.403478	0.505519	-1.321326
	6	-1.965016	-0.875666	-1.129433
	7	-0.602348	-1.183746	-1.172711
	6	-3.721832	0.752622	-1.714879
	6	-4.557206	-0.279512	-2.067117
	6	-4.097858	-1.620483	-2.046091
	6	-2.842615	-1.911742	-1.633001
	1	1.073769	2.502198	0.298378
	1	1.205430	2.766956	-1.430223
	1	2.113177	-2.309007	-1.152373
	1	4.581714	-1.854820	-0.952260
	1	5.385815	0.434767	-0.609813
	1	-1.785866	2.567640	-1.120396
	1	-4.064210	1.772056	-1.776979
	1	-5.560787	-0.068622	-2.392836
	1	-4.751331	-2.406531	-2.382780
	1	-2.460321	-2.916355	-1.619379
	8	-2.160709	-1.069763	0.627518
	6	-3.410453	-0.795654	1.176179
	1	-4.208981	-1.372595	0.712824
	1	-3.665733	0.262104	1.141704
	1	-3.345363	-1.099502	2.219865
TS10	Atomic			
	Number	X	Y	Z
	6	1.533332	-0.266929	0.126164
	7	0.559458	-1.195444	0.047349
	6	-0.571781	-0.501399	0.007588
	6	-0.422070	0.862938	0.060485
	6	0.958961	1.108614	0.135578
	6	-1.987185	-0.829619	-0.019752

	7	-2.643033	0.378500	0.007845
	6	-1.745277	1.541602	0.070581
	6	-2.670048	-1.994516	-0.073634
	6	-4.083398	-1.913188	-0.103667
	6	-4.729592	-0.722269	-0.080395
	6	-4.013955	0.527074	-0.022285
	6	2.953224	-0.627834	0.017172
	6	3.990920	0.244483	-0.124860
	6	4.008507	1.655928	-0.190386
	6	2.966930	2.592717	-0.125928
	6	1.627336	2.388434	0.025008
	8	-4.512742	1.640912	0.004063
	1	1.327032	0.444227	1.229782
	1	-1.927697	2.188910	-0.781193
	1	-1.949946	2.112846	0.970538
	1	-2.148369	-2.931643	-0.094522
	1	-4.657088	-2.823821	-0.146523
	1	-5.801750	-0.657416	-0.101823
	8	3.107908	-1.955612	0.087214
	1	4.966408	-0.201572	-0.192433
	1	4.991275	2.077573	-0.314445
	1	3.275430	3.622443	-0.207264
	1	0.978031	3.245644	0.059304
	6	4.388350	-2.526587	-0.050113
	1	4.240016	-3.594968	0.009765
	1	5.049738	-2.208284	0.750915
	1	4.828679	-2.275401	-1.010794
TS11	Atomic			
	Number	X	Y	Z
	6	-1.725266	1.275851	1.122513
	7	-0.518868	1.829346	1.400781
	6	0.371942	0.949547	0.966358
	6	-0.155669	-0.192164	0.401900
	6	-1.545210	-0.049143	0.474509
	6	1.821228	0.841573	0.997064
	7	2.110921	-0.378092	0.433809
	6	0.921690	-1.142965	0.024734
	6	2.802150	1.663502	1.431609
	6	4.135857	1.214007	1.276724
	6	4.422141	0.013714	0.716870
	6	3.385402	-0.872270	0.250710
	6	-2.946514	2.045873	1.248559
	6	-4.188739	1.674611	0.831199
	6	-4.613264	0.492225	0.198108

	6	-3.889359	-0.647036	-0.216209
	6	-2.558710	-0.917934	-0.110807
	8	3.553780	-1.967695	-0.260845
	8	-1.981348	-2.058954	-0.537553
	6	-2.756655	-3.035233	-1.198211
	1	-1.790664	0.150159	1.789295
	1	0.973892	-1.364751	-1.035353
	1	0.888354	-2.086739	0.558071
	1	2.563918	2.613168	1.870027
	1	4.941368	1.845008	1.613190
	1	5.432951	-0.330689	0.598899
	1	-2.812083	3.002639	1.720359
	1	-4.971557	2.393241	1.012472
	1	-5.666514	0.447904	-0.019864
	1	-4.492166	-1.406976	-0.680144
	1	-2.071375	-3.827546	-1.461937
	1	-3.207762	-2.630405	-2.099309
	1	-3.529670	-3.427878	-0.544229
TS12	Atomic			
	Number	X	Y	Z
	6	4.183699	-0.607083	1.088962
	6	4.375100	-1.726478	0.294235
	6	3.456337	-2.064305	-0.679039
	6	2.333362	-1.271322	-0.852008
	6	2.113983	-0.154969	-0.062805
	6	3.057330	0.182106	0.913011
	6	0.918639	0.689586	-0.276012
	6	-0.206296	0.621464	0.418847
	6	-1.425957	1.480039	0.196788
	7	-2.371931	0.994183	1.193198
	6	-1.885526	-0.006463	1.977498
	6	-2.629868	-0.569366	2.953233
	6	-3.944568	-0.071664	3.125931
	6	-4.432081	0.923535	2.347844
	6	-3.641611	1.529252	1.305257
	8	-3.997632	2.426475	0.562010
	6	-0.498351	-0.296615	1.547639
	7	0.238765	-1.159295	2.069076
	8	2.796198	1.292767	1.632644
	6	3.675395	1.658300	2.670415
	1	4.911953	-0.361024	1.838556
	1	5.252735	-2.331627	0.443824
	1	3.605202	-2.932909	-1.295668
	1	1.607506	-1.525470	-1.605827

	1	0.973426	1.417206	-1.074006
	1	-1.848259	1.367093	-0.795237
	1	-1.231663	2.534166	0.360875
	1	-2.230855	-1.357589	3.561587
	1	-4.567323	-0.497545	3.894267
	1	-5.428445	1.305470	2.473155
	1	3.257986	2.550553	3.115100
	1	4.668238	1.879456	2.287930
	1	3.740000	0.877678	3.423212
TS13	Atomic			
	Numbe	X	Y	Z
	6	2.100599	-0.786784	-1.383813
	7	1.235617	0.398429	-1.597506
	6	0.017171	-0.060635	-1.307430
	6	-0.052675	-1.457556	-1.079535
	6	1.199727	-1.949001	-1.130518
	6	-1.280806	0.517905	-1.146712
	7	-2.136907	-0.531363	-0.873143
	6	-1.467816	-1.839883	-0.806298
	6	-1.749988	1.791752	-1.228761
	6	-3.132813	1.988256	-1.023940
	6	-3.970126	0.953117	-0.758288
	6	-3.491089	-0.404845	-0.667131
	6	3.254648	-0.939980	-2.304370
	6	4.296854	-0.099123	-2.258965
	6	4.403703	0.915007	-1.248386
	6	3.497001	0.990895	-0.237730
	6	2.364488	0.147900	-0.205284
	8	-4.174282	-1.388720	-0.428239
	8	1.641868	0.047736	0.926972
	6	2.113619	-0.908518	1.866448
	1	1.543784	-2.957423	-1.002972
	1	-1.621906	-2.282265	0.171313
	1	-1.890732	-2.509637	-1.546956
	1	-1.081484	2.602823	-1.443721
	1	-3.531520	2.987237	-1.081513
	1	-5.022852	1.099632	-0.601957
	1	3.218161	-1.746020	-3.016281
	1	5.104175	-0.209751	-2.962803
	1	5.255295	1.572220	-1.255363
	1	3.633549	1.667413	0.588573
	1	1.408520	-0.903183	2.685947
	1	2.148647	-1.898788	1.422939
	1	3.098567	-0.634845	2.231426

TS14	Atomic Number	X	Y	Z
	6	-2.262117	-0.483593	-0.099099
	7	-1.175122	-0.680669	-1.077576
	6	-0.071819	-0.399469	-0.369432
	6	-0.320170	0.093996	0.935133
	6	-1.650471	0.079730	1.144948
	6	1.335029	-0.496800	-0.589882
	7	1.937189	-0.018522	0.559359
	6	0.981593	0.393552	1.599858
	6	2.089089	-0.927564	-1.638405
	6	3.491852	-0.860331	-1.499912
	6	4.077574	-0.384984	-0.370681
	6	3.296046	0.074117	0.752159
	6	-3.516094	0.109098	-0.642437
	6	-4.349626	-0.608584	-1.416734
	6	-4.106078	-2.000357	-1.665498
	6	-3.073372	-2.665818	-1.080623
	6	-2.152704	-1.972416	-0.271541
	8	3.742515	0.509229	1.802392
	8	-3.666303	1.387427	-0.280086
	6	-4.816169	2.080645	-0.715206
	1	-2.210661	0.372544	2.010771
	1	1.156822	-0.174159	2.506544
	1	1.117904	1.444063	1.832066
	1	1.618518	-1.294867	-2.529895
	1	4.112361	-1.194695	-2.314473
	1	5.145179	-0.332740	-0.263085
	1	-5.230243	-0.161411	-1.838313
	1	-4.801533	-2.531587	-2.291495
	1	-2.963747	-3.729302	-1.200254
	1	-1.464513	-2.490370	0.368283
	1	-4.743857	3.074220	-0.297547
	1	-4.842478	2.141950	-1.799116
	1	-5.718593	1.595668	-0.354227
TS15	Atomic Number	X	Y	Z
	6	1.820849	0.080897	-0.775026
	7	0.720423	0.979066	-0.967844
	6	-0.321038	0.305185	-0.590944
	6	-0.094457	-1.031047	-0.203234
	6	1.261754	-1.259969	-0.332192
	6	-1.739552	0.599293	-0.439120
	7	-2.313486	-0.552754	0.041366

	6	-1.361323	-1.655009	0.259580
	6	-2.478441	1.702609	-0.685738
	6	-3.869627	1.619264	-0.431686
	6	-4.436569	0.483057	0.038835
	6	-3.658229	-0.701700	0.307032
	6	2.943879	0.140222	-1.734166
	6	4.166998	-0.292689	-1.392988
	6	4.471675	-0.685179	-0.047220
	6	3.564569	-0.506172	0.957625
	6	2.247967	-0.074248	0.694774
	8	-4.090808	-1.760662	0.730781
	8	1.495459	0.441551	1.690067
	6	1.724533	1.822259	1.955586
	1	1.807929	-2.180400	-0.338590
	1	-1.354331	-1.929136	1.310053
	1	-1.674283	-2.524721	-0.308572
	1	-2.015898	2.594572	-1.061892
	1	-4.487840	2.481294	-0.617931
	1	-5.490596	0.414216	0.235433
	1	2.727667	0.526124	-2.714521
	1	4.959556	-0.291981	-2.121390
	1	5.463391	-1.030955	0.185574
	1	3.843806	-0.643403	1.988739
	1	1.530497	2.413063	1.067051
	1	1.032986	2.098092	2.739670
	1	2.743010	1.982664	2.295949
TS16	Atomic			
	Number	X	Y	Z
	6	-2.245441	-0.765637	1.685400
	6	-3.579892	-1.173753	1.868256
	6	-1.870913	0.038710	0.465793
	6	-4.547819	-0.790434	0.986403
	6	-3.021211	0.560343	-0.318105
	6	-4.272383	0.112279	-0.092637
	6	0.024687	-1.231269	0.302887
	6	-1.350159	-1.349917	0.168214
	6	1.287092	-2.016448	0.301127
	6	0.286903	0.118792	0.605840
	6	1.723244	0.282784	0.788678
	7	-0.742252	0.905969	0.683184
	7	2.272323	-0.962484	0.596379
	6	2.495139	1.354148	1.071951
	6	3.621726	-1.238630	0.662088
	6	4.434751	-0.086430	0.964611

	6	3.892720	1.139649	1.157510
	8	4.029662	-2.373375	0.475703
	8	-2.644922	1.426962	-1.256597
	6	-3.638260	2.020839	-2.063989
	1	-1.531982	-0.805842	2.485755
	1	-3.832862	-1.750631	2.740836
	1	-5.563771	-1.113465	1.131367
	1	-5.091295	0.445871	-0.701874
	1	-1.935970	-2.140316	-0.254208
	1	1.332137	-2.783965	1.068052
	1	1.527715	-2.484560	-0.647827
	1	2.051782	2.319881	1.219388
	1	5.493781	-0.255417	1.030063
	1	4.536718	1.973304	1.381692
	1	-3.121255	2.708621	-2.716904
	1	-4.154209	1.271820	-2.658057
	1	-4.355787	2.562605	-1.454983
TS17	Atomic Number	X	Y	Z
	6	-0.112391	0.022949	-0.147122
	6	-0.126386	0.037856	1.300181
	6	1.000741	0.085702	2.013534
	6	2.317821	0.018972	1.371706
	6	2.331792	-0.031156	-0.150306
	6	1.032560	0.053755	-0.831244
	7	2.628589	-1.260996	0.661590
	6	3.981708	-1.463799	0.410605
	6	4.538033	-0.558767	-0.495281
	6	3.584229	0.335804	-0.862811
	6	4.954506	-2.388740	0.849534
	7	6.133075	-2.042399	0.206230
	6	5.983878	-0.879718	-0.680144
	6	4.923321	-3.454773	1.705569
	6	6.122111	-4.170278	1.895796
	6	7.272731	-3.823438	1.259794
	6	7.328241	-2.702569	0.349321
	8	8.318647	-2.331990	-0.260931
	1	-1.053228	0.064007	-0.668361
	1	-1.077494	0.096373	1.801121
	1	0.975995	0.238868	3.079048
	1	1.038077	0.156796	-1.902868
	1	3.658140	1.166531	-1.537405
	1	6.650354	-0.084410	-0.365046

	1	6.245036	-1.152778	-1.696626
	1	4.009342	-3.729709	2.195877
	1	6.123618	-5.016295	2.562552
	1	8.187588	-4.368074	1.402827
	8	3.328384	0.670781	2.008370
	6	3.771721	0.108202	3.237082
	1	3.155142	-0.732653	3.535550
	1	4.795442	-0.228853	3.124577
	1	3.727150	0.874984	4.001102
TS18	Atomic Number	X	Y	Z
	6	1.915949	0.455910	-0.572967
	7	1.091967	1.587780	-0.525026
	6	-0.131471	1.221649	-0.330664
	6	-0.399941	-0.164400	-0.318453
	6	0.751226	-0.956664	-0.308552
	6	-1.392957	1.942525	-0.282402
	7	-2.378983	0.987758	-0.333614
	6	-1.869085	-0.387769	-0.392722
	6	-1.696449	3.258554	-0.229639
	6	-3.069351	3.605204	-0.228261
	6	-4.041516	2.662777	-0.280151
	6	-3.731461	1.256174	-0.342274
	6	2.940251	0.385339	-1.579944
	6	3.901729	-0.551713	-1.530573
	6	3.965491	-1.467134	-0.420447
	6	3.069140	-1.425584	0.569669
	6	1.922486	-0.490739	0.567543
	8	-4.539931	0.343718	-0.397246
	8	1.624710	0.048293	1.809421
	6	0.967622	-0.808967	2.714391
	1	0.800996	-1.948580	-0.719790
	1	-2.268838	-0.964327	0.435168
	1	-2.194753	-0.867033	-1.312277
	1	-0.917938	3.995473	-0.188507
	1	-3.344507	4.645554	-0.183340
	1	-5.084214	2.921820	-0.277287
	1	2.906514	1.125038	-2.360084
	1	4.656861	-0.597535	-2.295111
	1	4.784884	-2.163659	-0.370063
	1	3.174053	-2.064019	1.429797
	1	0.762707	-0.222093	3.599266
	1	0.030809	-1.173529	2.301679

	1	1.588000	-1.657823	2.992464
TS19	Atomic Number	X	Y	Z
	6	4.270200	0.172291	-0.234153
	6	4.295111	1.250127	0.727925
	6	3.317972	1.441336	1.614962
	6	2.135447	0.557109	1.622348
	6	2.181625	-0.603579	0.727699
	6	3.261867	-0.725339	-0.225006
	7	1.095819	0.905126	0.621801
	6	-0.062924	0.238837	0.804600
	6	-0.051118	-1.146173	1.090221
	6	1.189582	-1.659363	0.927092
	6	-1.408788	0.643246	0.558690
	7	-2.213084	-0.449209	0.814509
	6	-1.454424	-1.641486	1.212095
	6	-1.953703	1.831367	0.168629
	6	-3.356589	1.889888	0.038210
	6	-4.142441	0.814138	0.304805
	6	-3.583928	-0.449570	0.728989
	8	-4.223727	-1.455492	0.991837
	8	3.141165	-1.787415	-1.035991
	6	4.159106	-2.029701	-1.981365
	1	5.073521	0.097972	-0.942161
	1	5.152960	1.901130	0.722665
	1	3.375176	2.223781	2.351256
	1	1.721975	0.375942	2.607489
	1	1.453817	-2.697079	0.852014
	1	-1.735418	-1.932708	2.219051
	1	-1.684226	-2.466987	0.548338
	1	-1.321798	2.676080	-0.026920
	1	-3.814250	2.812614	-0.276816
	1	-5.211921	0.854865	0.210903
	1	3.871811	-2.927772	-2.508567
	1	5.116181	-2.184664	-1.491016
	1	4.238007	-1.205311	-2.684133
TS20	Atomic Number	X	Y	Z
	6	-2.206057	-0.877284	1.604292
	6	-3.601727	-1.328035	1.702740
	6	-1.931701	0.173884	0.614375
	6	-4.521202	-0.893935	0.833891

	6	-2.976444	0.594021	-0.295897
	6	-4.218080	0.062029	-0.198332
	6	0.001132	-1.269447	0.495574
	6	-1.346034	-1.592759	0.532850
	6	1.280767	-1.960707	0.176864
	6	0.255113	0.101388	0.742194
	6	1.692428	0.315111	0.742966
	7	-0.755259	0.912274	0.737654
	7	2.258627	-0.887932	0.399719
	6	2.457130	1.406708	0.973334
	6	3.612449	-1.104596	0.253373
	6	4.416133	0.064273	0.508976
	6	3.858328	1.252117	0.847847
	8	4.029167	-2.206914	-0.064985
	8	-2.582104	1.506355	-1.185613
	6	-3.532792	2.019699	-2.091955
	1	-1.688981	-0.772590	2.548730
	1	-3.863878	-2.001045	2.500315
	1	-5.537451	-1.241711	0.910951
	1	-4.997600	0.353911	-0.875567
	1	-1.801896	-2.410936	0.005801
	1	1.501501	-2.798565	0.829612
	1	1.346855	-2.315943	-0.848003
	1	2.003814	2.342373	1.237633
	1	5.479315	-0.057474	0.413915
	1	4.495154	2.102058	1.027490
	1	-3.009665	2.751748	-2.689560
	1	-3.919923	1.234539	-2.735331
	1	-4.353119	2.498386	-1.564854
TS21	Atomic Number	X	Y	Z
	6	-1.796404	-1.083038	-0.239013
	7	-0.671667	-1.673186	0.347132
	6	0.349793	-0.900602	-0.000826
	6	0.037162	0.175807	-0.793890
	6	-1.418725	0.187498	-0.962600
	6	1.782445	-0.921833	0.242246
	7	2.286050	0.156197	-0.446918
	6	1.260058	0.938358	-1.148672
	6	2.593196	-1.744152	0.942802
	6	3.978370	-1.446493	0.932510
	6	4.474464	-0.385675	0.251322
	6	3.620375	0.499874	-0.500196

	6	-2.951136	-1.869552	-0.542450
	6	-4.170115	-1.334980	-0.783847
	6	-4.486413	0.001300	-0.420860
	6	-3.599986	0.821272	0.203346
	6	-2.200903	0.584965	0.272117
	8	3.978885	1.475914	-1.138637
	8	-1.526180	1.095311	1.337516
	6	-1.157781	2.459516	1.227338
	1	-1.876216	0.431649	-1.907983
	1	1.275758	1.965610	-0.797112
	1	1.473288	0.959425	-2.214177
	1	2.190401	-2.581349	1.479107
	1	4.651782	-2.082236	1.482331
	1	5.524121	-0.156736	0.243438
	1	-2.809014	-2.936694	-0.547202
	1	-4.974514	-1.979436	-1.093407
	1	-5.517990	0.305777	-0.472394
	1	-3.965863	1.669569	0.758765
	1	-0.499344	2.672352	2.058017
	1	-0.639392	2.653610	0.293612
	1	-2.032505	3.100957	1.287585
TS22	Atomic Number	X	Y	Z
	6	-2.077992	-1.223390	1.522595
	6	-3.449641	-1.491235	1.694135
	6	-1.754131	0.001669	0.177542
	6	-4.391868	-1.152448	0.766638
	6	-2.985445	0.450544	-0.424373
	6	-4.167210	-0.213018	-0.270459
	6	0.096498	-1.324004	0.344902
	6	-1.359482	-1.441304	0.216678
	6	1.320596	-2.144119	0.511342
	6	0.381276	0.006566	0.459824
	6	1.805011	0.178461	0.692996
	7	-0.667367	0.836192	0.362459
	7	2.328122	-1.093473	0.708966
	6	2.595134	1.261331	0.863512
	6	3.663473	-1.390765	0.883268
	6	4.494940	-0.226859	1.062878
	6	3.979075	1.026055	1.053030
	8	4.040844	-2.551115	0.879737
	8	-2.826178	1.559493	-1.160323
	6	-3.965916	2.207139	-1.679575

	1	-1.448766	-1.104173	2.388376
	1	-3.765506	-1.887516	2.645245
	1	-5.409089	-1.470052	0.923471
	1	-5.020739	0.101314	-0.841174
	1	-1.817757	-2.146750	-0.458025
	1	1.298237	-2.806505	1.372850
	1	1.578265	-2.746677	-0.354987
	1	2.177478	2.249340	0.849879
	1	5.544182	-0.407345	1.207034
	1	4.636269	1.868023	1.191904
	1	-3.607874	3.121753	-2.129988
	1	-4.450941	1.599775	-2.438475
	1	-4.674495	2.439091	-0.889880
TS23	Atomic			
	Number	X	Y	Z
	6	0.017375	-0.314591	-0.291077
	6	-0.280451	1.083281	-0.294100
	6	1.458492	-0.466277	-0.220652
	7	2.002497	0.789769	-0.206844
	6	1.002825	1.855414	-0.268079
	6	2.240088	-1.571990	-0.174375
	6	3.638256	-1.370313	-0.109580
	6	4.175242	-0.125150	-0.095880
	6	3.352511	1.059573	-0.148165
	8	3.753241	2.211175	-0.144978
	6	-1.560684	1.477432	-0.303053
	6	-2.584589	0.447162	-0.222443
	6	-2.140789	-0.919359	-0.496898
	7	-0.847520	-1.280028	-0.415547
	6	-3.936778	0.782304	-0.622790
	6	-4.805927	-0.176445	-1.010075
	6	-4.391911	-1.533740	-1.098075
	6	-3.095990	-1.889573	-0.844844
	8	-2.726561	0.455619	1.563473
	6	-3.563246	-0.503143	2.133842
	1	1.096116	2.500193	0.598591
	1	1.160606	2.460179	-1.154807
	1	1.796978	-2.548814	-0.186431
	1	4.289299	-2.227252	-0.070060
	1	5.236666	0.033987	-0.046593
	1	-1.860921	2.511057	-0.296696
	1	-4.236731	1.813562	-0.552570
	1	-5.817545	0.083472	-1.269409

	1	-5.104496	-2.282884	-1.396299
	1	-2.761993	-2.906277	-0.953766
	1	-4.575778	-0.468678	1.735540
	1	-3.613819	-0.254866	3.192854
	1	-3.172362	-1.514000	2.036084
TS24	Atomic Number	X	Y	Z
	6	-1.894266	0.925617	-0.476450
	7	-1.115047	-0.283602	-0.747257
	6	0.197830	0.114679	-0.493434
	6	0.293030	1.447451	-0.126602
	6	-0.968050	1.980145	-0.079006
	6	1.464015	-0.513106	-0.457351
	7	2.361742	0.473613	-0.083399
	6	1.721576	1.774157	0.152944
	6	1.898489	-1.782262	-0.710690
	6	3.279239	-2.032435	-0.577298
	6	4.154150	-1.057742	-0.213708
	6	3.715880	0.290924	0.056735
	6	-3.127636	1.154144	-1.173755
	6	-4.061939	0.193780	-1.353017
	6	-4.045120	-1.025835	-0.622213
	6	-3.102086	-1.311246	0.307884
	6	-1.891186	-0.570334	0.435165
	8	4.434902	1.221733	0.386306
	8	-1.178666	-0.639665	1.577730
	6	-1.838946	-0.230580	2.763751
	1	-1.267212	2.982004	0.160365
	1	1.902462	2.097450	1.172267
	1	2.140026	2.520845	-0.513336
	1	1.204934	-2.546116	-1.004853
	1	3.649022	-3.025418	-0.771183
	1	5.206513	-1.247657	-0.112185
	1	-3.313968	2.157873	-1.518321
	1	-4.934661	0.415790	-1.942805
	1	-4.904367	-1.670233	-0.699116
	1	-3.276047	-2.084253	1.037852
	1	-1.100925	-0.279411	3.552093
	1	-2.200392	0.787866	2.658167
	1	-2.666768	-0.888342	3.005482
TS25	Atomic Number	X	Y	Z

	6	-1.853827	0.234738	-0.087444
	7	-0.838525	-0.209960	-1.008041
	6	0.350512	0.088600	-0.345340
	6	0.136331	0.697906	0.875621
	6	-1.221086	0.798267	1.087368
	6	1.734267	-0.116673	-0.577580
	7	2.378102	0.405761	0.531348
	6	1.452070	0.964123	1.525822
	6	2.451001	-0.673925	-1.594947
	6	3.855728	-0.688697	-1.463974
	6	4.481404	-0.170694	-0.375057
	6	3.741097	0.425847	0.710923
	6	-3.141324	0.613561	-0.600669
	6	-3.771989	-0.066159	-1.601419
	6	-3.419849	-1.385034	-1.968615
	6	-2.423460	-2.089372	-1.353436
	6	-1.438927	-1.458677	-0.578894
	8	4.223508	0.914596	1.720504
	8	-3.656405	1.678973	0.045072
	6	-5.000433	2.036005	-0.189912
	1	-1.748450	1.226214	1.914930
	1	1.579210	0.459524	2.477403
	1	1.660202	2.017964	1.676704
	1	1.953290	-1.071875	-2.458119
	1	4.446532	-1.122544	-2.253325
	1	5.550944	-0.181418	-0.275438
	1	-4.681741	0.331868	-2.011206
	1	-4.092061	-1.904062	-2.630833
	1	-2.443420	-3.166457	-1.359481
	1	-0.874035	-2.010444	0.153868
	1	-5.226170	2.827748	0.510236
	1	-5.136200	2.405231	-1.202180
	1	-5.662296	1.192066	-0.017890

Table AP6. Calculated geometries of stationary points on the deiodination and Diels-Alder cycloaddition-elimination pathways using the BH*and*HLYP methods with the 6-311++G(d,p) (for the C, H, N, and O atoms) and LANL2DZ (for the Sn and I atoms) basis sets.

Species	Geometries			
1b	Atomic			
	Number	X	Y	Z
	6	-4.448420	0.662267	-0.014366
	6	-4.860783	-0.658488	-0.108489
	6	-3.966859	-1.670949	0.210265
	6	-2.675778	-1.388154	0.602725
	6	-2.258392	-0.061324	0.686802
	6	-3.154211	0.954175	0.397231
	6	-0.910228	0.308898	1.144611
	6	0.276855	-0.098815	0.734397
	6	1.547044	0.356433	1.393119
	7	2.440599	1.087978	0.494556
	6	3.598499	0.537725	0.005061
	6	4.401478	1.200847	-0.855806
	6	4.025714	2.505047	-1.264689
	6	2.909028	3.073750	-0.774570
	6	2.056947	2.390854	0.171325
	8	1.069222	2.879364	0.678268
	6	3.993386	-0.756443	0.466737
	7	4.361724	-1.772484	0.831943
	8	-5.231699	1.726487	-0.291983
	1	-5.858751	-0.909244	-0.415317
	1	-4.293800	-2.694927	0.151217
	1	-2.000882	-2.184461	0.856466
	1	-2.859003	1.986369	0.473126
	1	-0.885584	1.062784	1.918939
	1	2.090950	-0.487989	1.794583
	1	1.291786	1.018512	2.209847
	1	5.303033	0.737653	-1.206481
	1	4.648213	3.037487	-1.962421
	1	2.600258	4.065059	-1.050433
	3	0.553051	-1.422770	-0.912470
	6	-6.557659	1.504628	-0.708057
	1	-6.988838	2.482227	-0.870808
	1	-6.590845	0.939155	-1.635659
	1	-7.129233	0.983141	0.055290
·Sn(CH$_3$)$_3$	Atomic			

	Number	X	Y	Z
	50	-0.928902	0.701476	0.419032
	6	-2.597484	-0.551442	-0.124330
	6	0.454445	-0.483334	1.572562
	6	0.063937	1.321867	-1.391504
	1	-2.236265	-1.403826	-0.693802
	1	-3.307622	-0.003484	-0.733551
	1	-3.108122	-0.916623	0.759762
	1	1.329162	0.098848	1.840248
	1	0.773542	-1.338564	0.982622
	1	-0.013355	-0.844544	2.481633
	1	0.932353	1.930323	-1.164899
	1	-0.607061	1.895744	-2.020907
	1	0.389571	0.442858	-1.941566
TS2 (Singlet)	Atomic Number	X	Y	Z
	6	-3.389444	-0.887178	-0.313331
	6	-4.404805	-0.851134	0.595579
	6	-4.288485	-0.035974	1.740507
	6	-3.184866	0.728645	1.973888
	6	-2.119648	0.696046	1.064639
	6	-2.193141	-0.115697	-0.095064
	7	-0.263901	-0.326168	2.018221
	6	0.530443	-0.416480	1.128114
	6	0.231217	0.036637	-0.562657
	6	-1.077216	-0.373807	-0.869478
	6	1.914021	-0.902887	1.017416
	7	2.339341	-0.999505	-0.267979
	6	1.359376	-0.653422	-1.291643
	6	2.714582	-1.238332	2.052396
	6	4.021484	-1.686033	1.745514
	6	4.448602	-1.786911	0.465281
	6	3.592513	-1.454415	-0.643506
	8	3.879696	-1.547048	-1.824575
	8	-3.392963	-1.621432	-1.431694
	1	-5.296546	-1.431011	0.454461
	1	-5.114990	-0.006420	2.430281
	1	-3.128501	1.368281	2.835373
	1	-1.380289	1.465101	1.120079
	3	0.647611	2.193838	-0.502501
	1	-1.171576	-1.163287	-1.595857
	1	1.843912	-0.052867	-2.046859
	1	1.001718	-1.564660	-1.762902

	1	2.355943	-1.151316	3.059226
	1	4.686279	-1.950329	2.550443
	1	5.437443	-2.127427	0.219347
	6	-4.499003	-2.455771	-1.704370
	1	-4.275088	-2.950982	-2.637809
	1	-5.407328	-1.871082	-1.812918
	1	-4.628891	-3.196072	-0.920900
8	Atomic Numbe	X	Y	Z
	6	3.463548	-0.467329	0.576054
	6	4.323591	-1.182106	-0.165707
	6	3.877009	-1.867586	-1.366805
	6	2.642496	-1.741954	-1.837139
	6	1.662026	-0.815457	-1.195522
	6	2.064276	-0.349751	0.186725
	7	0.309282	-1.351765	-1.269623
	6	-0.527781	-0.833831	-0.493031
	6	-0.248684	0.215565	0.536775
	6	1.141870	0.186127	0.988719
	6	-1.936158	-1.218950	-0.345369
	7	-2.395662	-0.658319	0.810281
	6	-1.362639	0.050843	1.559405
	6	-2.729437	-1.974079	-1.130973
	6	-4.069618	-2.154375	-0.705243
	6	-4.526595	-1.603274	0.443714
	6	-3.675516	-0.816672	1.303590
	8	-3.993227	-0.321321	2.370288
	8	3.747253	0.150435	1.734999
	1	5.348130	-1.297409	0.133759
	1	4.586362	-2.500843	-1.871723
	1	2.311983	-2.255737	-2.722377
	1	1.637910	0.093200	-1.818194
	53	-0.628730	2.153231	-0.569706
	1	1.392703	0.576882	1.957581
	1	-1.758880	0.967996	1.965162
	1	-1.020280	-0.571870	2.382678
	1	-2.348990	-2.400644	-2.038642
	1	-4.736793	-2.742574	-1.312282
	1	-5.540560	-1.737419	0.772809
	6	5.052261	0.038678	2.254689
	1	5.055723	0.593622	3.181711
	1	5.780735	0.468261	1.572733
	1	5.304422	-0.999837	2.450499

TS3

Atomic Number	X	Y	Z
6	3.383009	-0.829085	0.470312
6	4.265663	-0.933752	-0.555747
6	3.830360	-0.953123	-1.921233
6	2.538106	-0.837045	-2.245965
6	1.533480	-0.593416	-1.205354
6	1.985378	-0.715966	0.200023
7	0.221554	-1.084034	-1.510330
6	-0.609748	-0.881069	-0.578285
6	-0.267788	-0.375238	0.746933
6	1.038321	-0.551572	1.180725
6	-2.052015	-1.129145	-0.589815
7	-2.534099	-0.798035	0.644034
6	-1.507767	-0.354481	1.582827
6	-2.860704	-1.583140	-1.568071
6	-4.239632	-1.695643	-1.260410
6	-4.720454	-1.367659	-0.038092
6	-3.859176	-0.893387	1.018084
8	-4.201884	-0.597519	2.148839
8	3.696058	-0.835072	1.774502
6	5.051635	-0.955292	2.149190
1	5.064985	-0.938543	3.228942
1	5.317904	-1.019521	-0.358532
1	4.575244	-1.081323	-2.686689
1	2.194469	-0.870011	-3.263966
1	1.337820	0.552029	-1.214081
53	-0.251536	2.237759	-0.275706
1	1.306682	-0.502645	2.219118
1	-1.752469	0.618957	1.983999
1	-1.431431	-1.054957	2.409851
1	-2.462075	-1.830769	-2.532662
1	-4.917412	-2.049240	-2.018741
1	-5.764515	-1.451184	0.201430
1	5.634928	-0.122763	1.766615
1	5.470978	-1.892823	1.795401

2b

Atomic Number	X	Y	Z
6	-1.435321	2.117931	-3.046111
6	-0.594922	1.173623	-3.671718
6	-0.011631	0.164478	-2.973330
6	-0.245565	0.047945	-1.584447
6	-1.088043	0.988090	-0.936483

	6	-1.679285	2.029963	-1.705132
	7	0.347505	-0.965929	-0.913380
	6	0.108377	-1.039418	0.360239
	6	-0.709217	-0.161497	1.099377
	6	-1.315968	0.864493	0.448925
	6	0.638887	-2.045548	1.278154
	7	0.140886	-1.757373	2.517849
	6	-0.728957	-0.582929	2.534435
	6	1.461642	-3.098770	1.077895
	6	1.782448	-3.887032	2.208773
	6	1.288529	-3.601297	3.438544
	6	0.410728	-2.480585	3.661776
	8	-0.079343	-2.149239	4.728728
	8	-2.462085	2.874008	-1.008584
	6	-3.089963	3.937652	-1.688094
	1	-1.874442	2.898305	-3.638003
	1	-0.419178	1.265705	-4.729649
	1	0.629661	-0.558090	-3.444363
	1	-1.952670	1.571810	0.948852
	1	-1.716010	-0.858323	2.891062
	1	-0.328227	0.165013	3.210673
	1	1.843365	-3.310429	0.098104
	1	2.435633	-4.734678	2.086572
	1	1.530132	-4.197700	4.299021
	1	-3.658109	4.475325	-0.942781
	1	-3.761552	3.567107	-2.457268
	1	-2.356306	4.603388	-2.133637
HI	Atomic Number	X	Y	Z
	1	0.000000	0.000000	0.042961
	53	0.000000	0.000000	1.637039
$ISn(CH_3)_3$	Atomic Number	X	Y	Z
	6	1.119137	1.442404	1.795111
	1	0.704334	2.442068	1.763886
	1	0.701487	0.917358	2.644962
	1	2.195623	1.505206	1.907122
	6	1.118994	-1.676174	-0.005298
	1	0.703909	-2.149127	0.875808
	1	0.701592	-2.149412	-0.885157
	1	2.195474	-1.804709	-0.006848
	6	1.119466	1.442350	-1.805618

	1	0.704247	0.915999	-2.655874
	1	0.702491	2.441120	-1.775480
	1	2.195966	1.507436	-1.916150
	50	0.616732	0.402715	-0.005231
	53	-2.234539	0.402911	-0.005068
3b	Atomic Number	X	Y	Z
	6	-4.483783	0.287362	0.575302
	6	-4.415153	1.622459	0.936909
	6	-3.241492	2.334889	0.769348
	6	-2.135555	1.699818	0.237854
	6	-2.171551	0.361001	-0.132457
	6	-3.369976	-0.345675	0.041659
	6	-1.001181	-0.318286	-0.695668
	6	0.188624	0.199939	-0.875139
	6	1.470441	-0.243939	-1.443899
	7	2.538984	-0.325735	-0.438945
	6	3.240940	0.790281	-0.067496
	6	4.203191	0.755962	0.881176
	6	4.482216	-0.483211	1.510006
	6	3.799167	-1.589839	1.162712
	6	2.760593	-1.566726	0.157529
	8	2.111777	-2.537743	-0.172899
	6	2.940149	2.025464	-0.721565
	7	2.730179	3.027072	-1.225696
	8	-3.361617	-1.642078	-0.335022
	6	-4.526863	-2.415527	-0.173801
	1	-5.403489	-0.249533	0.711294
	1	-5.286787	2.101137	1.349156
	1	-3.187765	3.372598	1.047723
	1	-1.217650	2.245595	0.100327
	1	-1.144822	-1.353274	-0.982688
	1	1.798206	0.420782	-2.234958
	1	1.363075	-1.240234	-1.860449
	1	4.732787	1.652657	1.137861
	1	5.245526	-0.529152	2.267102
	1	3.983066	-2.544359	1.620061
	1	-4.279942	-3.405087	-0.531300
	1	-4.819470	-2.473676	0.870963
	1	-5.349587	-2.016355	-0.760723
TS1	Atomic Number	X	Y	Z

	6	4.704179	-2.689939	0.469308
	6	4.063868	-3.749841	-0.154926
	6	3.015652	-3.522294	-1.024219
	6	2.599073	-2.222295	-1.259307
	6	3.207218	-1.143863	-0.636663
	6	4.285807	-1.391242	0.224278
	6	2.819275	0.245574	-0.911111
	6	1.621877	0.791588	-0.969147
	6	1.361820	2.195373	-1.409724
	7	0.653123	3.011173	-0.419163
	6	-0.674403	3.324912	-0.549961
	6	-1.348181	4.022849	0.391381
	6	-0.649120	4.442819	1.550288
	6	0.661756	4.170821	1.685453
	6	1.401729	3.449693	0.674167
	8	2.591735	3.225407	0.732051
	6	-1.358531	2.947692	-1.747852
	7	-1.943127	2.696991	-2.694961
	1	5.521609	-2.884631	1.137835
	1	4.398699	-4.754294	0.040372
	1	2.529015	-4.342996	-1.521175
	1	1.797733	-2.035601	-1.950775
	1	3.647738	0.924699	-1.073364
	1	0.776968	2.200263	-2.320272
	1	2.309356	2.680846	-1.612172
	1	-2.384383	4.255486	0.241602
	1	-1.175294	4.988140	2.314409
	1	1.228161	4.484038	2.542993
	3	-0.316821	-0.325722	-0.350617
	0	-3.176227	-1.420244	0.437512
	6	-4.308868	0.392883	0.721280
	6	-3.022689	-2.562590	2.261292
	6	-3.934132	-2.597338	-1.202396
	1	-3.894670	0.957287	1.547784
	1	-5.345624	0.156197	0.937043
	1	-4.264266	0.997225	-0.176392
	1	-4.012722	-2.856660	2.594702
	1	-2.552293	-1.965021	3.032083
	1	-2.426308	-3.450647	2.093321
	1	-4.943001	-2.929435	-0.979550
	1	-3.303126	-3.463023	-1.360361
	1	-3.948631	-2.002115	-2.106765
	8	4.854557	-0.302168	0.777409
	6	5.941272	-0.461908	1.656605

	1	6.224481	0.534621	1.964062
	1	5.657392	-1.040457	2.531640
	1	6.783019	-0.940103	1.162381

Table AP7. Calculated geometries of stationary points on the radical oxidation pathways by $\cdot CH_3$ and $\cdot Sn(CH_3)_3$ using the BH*and*HLYP methods with the 6-311++G(d,p) (for the C, H, N, and O atoms) and LANL2DZ (for the Sn atom) basis sets.

Species	Geometries			
TS24–CH3	Atomic			
(Triplet)	Number	X	Y	Z
	6	4.196362	0.729264	0.437624
	6	3.685735	2.083670	0.295553
	6	2.401992	2.376506	0.534109
	6	1.499664	1.354991	1.046547
	6	1.935612	-0.071882	0.825400
	6	3.364816	-0.298375	0.685238
	7	0.088733	1.679197	0.911298
	6	-0.699020	0.672405	0.815933
	6	-0.341270	-0.705998	0.793354
	6	1.019914	-1.071401	0.772827
	6	-2.161564	0.740731	0.705447
	7	-2.626876	-0.541663	0.638563
	6	-1.565015	-1.545263	0.686275
	6	-3.002404	1.797167	0.671820
	6	-4.385665	1.515062	0.563231
	6	-4.847479	0.242577	0.498217
	6	-3.957489	-0.890973	0.535077
	8	-4.284765	-2.065082	0.482936
	8	3.713831	-1.594835	0.755214
	6	5.061226	-1.941677	0.533107
	1	5.246738	0.563995	0.287885
	1	4.373885	2.851400	-0.012258
	1	2.017829	3.376702	0.438277
	1	1.330068	-2.095814	0.676802
	1	-1.716707	-2.206665	1.535643
	1	-1.593168	-2.158976	-0.210479
	1	-2.618077	2.797202	0.725954
	1	-5.085532	2.333161	0.532144
	1	-5.896157	0.023332	0.416123
	1	5.114355	-3.017131	0.623022
	1	5.380478	-1.642734	-0.461504
	1	5.708757	-1.484076	1.275922
	6	1.559582	1.405080	3.739871
	1	2.596984	1.307969	4.022201
	1	1.113109	2.360084	3.970153
	1	0.944337	0.549634	3.972311
	1	1.620217	1.427477	2.356669

TS25–CH3 (Triplet)	Atomic Number	X	Y	Z
	6	4.124421	-1.562670	0.289392
	6	4.196092	-0.125563	0.421171
	6	3.097265	0.617305	0.658639
	6	1.785363	-0.029367	0.770570
	6	1.800344	-1.513487	0.992600
	6	2.984816	-2.225320	0.518163
	7	0.723287	0.688185	0.712420
	6	-0.472670	0.020607	0.711301
	6	-0.610526	-1.400929	0.706441
	6	0.470815	-2.180159	0.813539
	6	-1.745047	0.609295	0.638182
	7	-2.685604	-0.401783	0.578575
	6	-2.071656	-1.728085	0.584754
	6	-2.145237	1.926423	0.622128
	6	-3.522931	2.184873	0.550601
	6	-4.439760	1.176483	0.496056
	6	-4.040336	-0.214117	0.503342
	8	-4.800787	-1.168300	0.447397
	8	3.057488	1.950288	0.741546
	6	4.253505	2.669737	0.557383
	1	5.017105	-2.089912	0.001314
	1	5.151159	0.346439	0.285205
	1	2.935807	-3.297881	0.435487
	1	0.427958	-3.255821	0.820373
	1	-2.449472	-2.311091	1.417222
	1	-2.315641	-2.255526	-0.331487
	1	-1.410778	2.707129	0.664496
	1	-3.863567	3.206660	0.538504
	1	-5.494960	1.369614	0.440885
	1	3.993517	3.713635	0.656792
	1	4.667728	2.491011	-0.431411
	1	4.989840	2.406396	1.312427
	6	1.902694	-1.522777	3.725031
	1	1.634966	-2.542695	3.950453
	1	2.920891	-1.245295	3.947109
	1	1.152833	-0.781564	3.949909
	1	1.932244	-1.527106	2.262099
TS26–CH3 (Triplet)	Atomic Number	X	Y	Z
	6	-0.571276	0.818481	0.283757

	7	0.350534	0.155074	1.182406
	6	1.472619	0.202077	0.571987
	6	1.473973	0.895493	-0.679912
	6	0.196083	1.342635	-0.891101
	6	2.820278	-0.291111	0.824888
	7	3.579330	0.115471	-0.247255
	6	2.837457	0.876616	-1.269716
	6	3.360092	-0.998536	1.839913
	6	4.741261	-1.303742	1.754567
	6	5.489579	-0.902946	0.700037
	6	4.925314	-0.146315	-0.391847
	6	-1.599537	1.692169	0.931816
	6	-2.469628	2.472390	0.259213
	6	-2.543176	2.727562	-1.151649
	6	-1.600909	2.547522	-2.135330
	6	-0.315345	2.016952	-2.012771
	8	5.529719	0.249517	-1.374318
	1	-1.253428	-0.155559	-0.161848
	1	3.283722	1.858496	-1.389904
	1	2.902957	0.365001	-2.224752
	1	2.753536	-1.307094	2.669334
	1	5.202576	-1.866983	2.548076
	1	6.537142	-1.130759	0.628446
	1	-3.227984	2.968543	0.837025
	1	-3.455337	3.209645	-1.463244
	1	-1.866303	2.917688	-3.112508
	1	0.347396	2.122873	-2.855708
	8	-1.599387	1.546744	2.258353
	6	-2.499834	2.293714	3.044475
	1	-2.276437	2.038938	4.070342
	1	-2.357558	3.359607	2.892322
	1	-3.528738	2.026939	2.820390
	6	-2.057698	-1.279983	-0.562574
	1	-2.464502	-1.623469	0.374790
	1	-1.323524	-1.927745	-1.015012
	1	-2.761356	-0.824191	-1.240776
TS27–CH3 (Triplet)	Atomic Number	X	Y	Z
	6	0.453531	1.570339	0.030766
	7	-0.584850	1.826414	-0.707554
	6	-1.586196	0.982120	-0.242260
	6	-1.210884	0.191891	0.768456
	6	0.209063	0.461696	1.018002

	6	-2.966725	0.741430	-0.586894
	7	-3.385916	-0.241796	0.280943
	6	-2.332489	-0.677957	1.204211
	6	-3.813059	1.262936	-1.507056
	6	-5.132160	0.752604	-1.530143
	6	-5.542865	-0.215691	-0.673368
	6	-4.655004	-0.779266	0.310439
	6	1.725372	2.215981	-0.187096
	6	2.812481	2.155264	0.675410
	6	2.915835	1.630371	1.953499
	6	1.923029	0.998910	2.774773
	6	0.732748	0.509471	2.408862
	8	-4.934588	-1.650226	1.119914
	1	0.829182	-0.524112	0.478469
	1	-2.651681	-0.519206	2.230486
	1	-2.147955	-1.741345	1.080262
	1	-3.482419	2.028876	-2.181357
	1	-5.829144	1.146663	-2.250882
	1	-6.544713	-0.602897	-0.691789
	1	3.709731	2.632012	0.323281
	1	3.873423	1.770165	2.425886
	1	2.185323	0.907381	3.816765
	1	0.099237	0.076884	3.164985
	8	1.765077	2.892443	-1.346999
	6	2.870669	3.705706	-1.663202
	1	2.614360	4.201384	-2.588605
	1	3.046595	4.449192	-0.890991
	1	3.769821	3.114495	-1.813784
	6	1.580365	-1.626720	-0.030066
	1	2.591758	-1.342690	0.212718
	1	1.186712	-2.461533	0.527914
	1	1.327050	-1.606407	-1.078366
TS29–CH3 (Triplet)	Atomic Number	X	Y	Z
	6	-0.278519	0.446731	1.441434
	7	0.703356	-0.567417	1.739969
	6	1.732524	-0.223976	1.064960
	6	1.612038	1.009849	0.335920
	6	0.370391	1.490343	0.594498
	6	3.064527	-0.763697	0.832781
	7	3.698460	0.131341	0.003643
	6	2.877714	1.294971	-0.386532
	6	3.686388	-1.879584	1.271045

	6	5.019925	-2.089344	0.841636
	6	5.645620	-1.208199	0.026196
	6	4.992532	-0.011944	-0.449373
	6	-1.141371	0.826411	2.589813
	6	-1.973758	1.875554	2.626904
	6	-2.182641	2.896218	1.639366
	6	-1.414313	3.244949	0.540263
	6	-0.231234	2.678473	0.086021
	8	5.487561	0.826370	-1.183958
	1	3.367956	2.211170	-0.076872
	1	2.770642	1.325714	-1.464710
	1	3.176546	-2.566845	1.918198
	1	5.544292	-2.969678	1.172992
	1	6.656661	-1.360419	-0.303985
	1	-1.101907	0.153212	3.428764
	1	-2.584464	1.973206	3.510485
	1	-3.036428	3.528487	1.816391
	1	-1.767438	4.105894	0.001068
	8	0.500824	3.218678	-0.917541
	6	0.150685	4.472110	-1.458901
	1	-0.805311	4.428304	-1.972735
	1	0.117428	5.237305	-0.688711
	1	0.925541	4.712938	-2.172795
	1	-1.066407	-0.158290	0.660088
	6	-2.032045	-0.894428	-0.140479
	1	-2.813137	-0.164748	-0.281575
	1	-1.448506	-1.135128	-1.014917
	1	-2.275827	-1.724785	0.502009
TS28–CH3 (Triplet)	Atomic Numbe	X	Y	Z
	6	0.298760	1.241675	-1.698531
	7	-0.865599	0.901622	-2.213531
	6	-1.667612	0.568468	-1.134586
	6	-1.067552	0.676221	0.057133
	6	0.329670	1.060599	-0.209646
	6	-3.028174	0.110710	-0.972230
	7	-3.193636	-0.049831	0.384204
	6	-1.989102	0.288109	1.151917
	6	-4.041146	-0.149174	-1.832888
	6	-5.263923	-0.588088	-1.272820
	6	-5.425506	-0.744101	0.064890
	6	-4.357493	-0.470299	0.991527
	6	1.386089	1.615704	-2.515863

	6	2.614060	2.108031	-2.079088
	6	2.984847	2.524962	-0.819918
	6	2.220318	2.609429	0.393892
	6	1.043806	2.021142	0.673833
	8	-4.411425	-0.580997	2.206730
	8	0.378969	2.161243	1.830293
	6	0.882112	3.025748	2.827399
	1	-2.201433	1.089885	1.851000
	1	-1.660427	-0.571488	1.729093
	1	-3.907332	-0.021907	-2.889582
	1	-6.089253	-0.803791	-1.930733
	1	-6.354213	-1.077772	0.489443
	1	1.226686	1.500249	-3.573947
	1	3.361985	2.233993	-2.845347
	1	3.983980	2.919516	-0.737153
	1	2.667542	3.212619	1.163120
	1	0.164209	2.997494	3.634068
	1	0.969988	4.039742	2.449919
	1	1.847428	2.682363	3.186799
	1	0.985579	-0.037448	-0.053719
	6	1.741295	-1.211075	0.184041
	1	2.724233	-0.913417	-0.144746
	1	1.632870	-1.361061	1.246642
	1	1.239854	-1.933427	-0.440717
3b	Atomic Number	X	Y	Z
	6	-4.483783	0.287362	0.575302
	6	-4.415153	1.622459	0.936909
	6	-3.241492	2.334889	0.769348
	6	-2.135555	1.699818	0.237854
	6	-2.171551	0.361001	-0.132457
	6	-3.369976	-0.345675	0.041659
	6	-1.001181	-0.318286	-0.695668
	6	0.188624	0.199939	-0.875139
	6	1.470441	-0.243939	-1.443899
	7	2.538984	-0.325735	-0.438945
	6	3.240940	0.790281	-0.067496
	6	4.203191	0.755962	0.881176
	6	4.482216	-0.483211	1.510006
	6	3.799167	-1.589839	1.162712
	6	2.760593	-1.566726	0.157529
	8	2.111777	-2.537743	-0.172899
	6	2.940149	2.025464	-0.721565

	7	2.730179	3.027072	-1.225696
	8	-3.361617	-1.642078	-0.335022
	6	-4.526863	-2.415527	-0.173801
	1	-5.403489	-0.249533	0.711294
	1	-5.286787	2.101137	1.349156
	1	-3.187765	3.372598	1.047723
	1	-1.217650	2.245595	0.100327
	1	-1.144822	-1.353274	-0.982688
	1	1.798206	0.420782	-2.234958
	1	1.363075	-1.240234	-1.860449
	1	4.732787	1.652657	1.137861
	1	5.245526	-0.529152	2.267102
	1	3.983066	-2.544359	1.620061
	1	-4.279942	-3.405087	-0.531300
	1	-4.819470	-2.473676	0.870963
	1	-5.349587	-2.016355	-0.760723
6b	Atomic			
	Number	X	Y	Z
	6	4.148293	0.669153	-0.228574
	6	3.667686	2.021824	-0.267604
	6	2.402599	2.331789	0.034775
	6	1.464668	1.284263	0.532876
	6	1.909942	-0.127077	0.231873
	6	3.285911	-0.370097	-0.005577
	7	0.080921	1.604047	0.222138
	6	-0.715469	0.605389	0.196559
	6	-0.365743	-0.780985	0.298867
	6	0.956453	-1.141291	0.246268
	6	-2.169165	0.672599	0.000529
	7	-2.645494	-0.606750	0.033151
	6	-1.603729	-1.613723	0.233785
	6	-2.994829	1.726923	-0.175662
	6	-4.373988	1.445771	-0.327670
	6	-4.847557	0.176351	-0.292756
	6	-3.974481	-0.954019	-0.099631
	8	-4.312723	-2.125175	-0.050359
	8	3.633385	-1.673232	-0.050295
	6	4.958266	-2.015679	-0.385273
	1	5.182948	0.486129	-0.447641
	1	4.356857	2.792662	-0.567672
	1	2.033106	3.341217	0.000012
	1	1.512599	1.365513	1.637842
	1	1.263013	-2.167628	0.150486

	1	-1.802023	-2.170048	1.145143
	1	-1.607971	-2.320627	-0.589828
	1	-2.602241	2.724996	-0.195837
	1	-5.061267	2.262159	-0.473383
	1	-5.893376	-0.042395	-0.406498
	1	4.999320	-3.095532	-0.378519
	1	5.219173	-1.650086	-1.374570
	1	5.661757	-1.625182	0.344766
14	Atomic			
	Number	X	Y	Z
	6	4.055065	-1.560427	-0.361909
	6	4.126869	-0.125081	-0.241928
	6	3.023311	0.619218	0.026189
	6	1.744298	-0.027883	0.204578
	6	1.751651	-1.518041	0.483812
	6	2.944251	-2.234002	-0.066008
	7	0.654133	0.687672	0.163294
	6	-0.507673	0.034154	0.168040
	6	-0.650661	-1.383695	0.090949
	6	0.433134	-2.165438	0.173461
	6	-1.807272	0.632820	0.090576
	7	-2.723775	-0.381956	-0.044166
	6	-2.104893	-1.706175	-0.092322
	6	-2.208942	1.933558	0.130439
	6	-3.593551	2.185149	0.033137
	6	-4.494951	1.176734	-0.095895
	6	-4.083815	-0.205895	-0.145428
	8	-4.825761	-1.168010	-0.266685
	8	2.990814	1.956948	0.077398
	6	4.174239	2.671720	-0.186429
	1	4.932822	-2.080601	-0.705498
	1	5.070647	0.351080	-0.429554
	1	1.872055	-1.582961	1.583289
	1	2.896628	-3.306924	-0.142992
	1	0.390320	-3.239118	0.100985
	1	-2.507871	-2.332450	0.695583
	1	-2.323118	-2.182421	-1.042504
	1	-1.484789	2.718212	0.233925
	1	-3.942744	3.203678	0.062961
	1	-5.550219	1.363639	-0.170114
	1	3.917288	3.717638	-0.099488
	1	4.537743	2.470468	-1.190805
	1	4.950000	2.429969	0.535574

21	Atomic Number X Y Z 6 -1.802077 1.047580 1.507126 7 -0.493780 1.634917 1.803126 6 0.350157 0.848609 1.248360 6 -0.192200 -0.254539 0.518541 6 -1.545152 -0.150151 0.601474 6 1.804742 0.797107 1.140512 7 2.089089 -0.304013 0.369700 6 0.903766 -1.056932 -0.083104 6 2.783850 1.584754 1.632951 6 4.119497 1.228333 1.321041 6 4.401509 0.144221 0.560987 6 3.363185 -0.705469 0.028746 6 -2.759066 2.064347 0.971659 6 -3.964672 1.776438 0.456660 6 -4.527199 0.487333 0.198840 6 -3.897618 -0.727104 0.018389 6 -2.529449 -1.006579 0.070248 8 3.535338 -1.694906 -0.663243 8 -2.011589 -2.164441 -0.397116 6 -2.816135 -3.064814 -1.127451 1 -2.193691 0.672415 2.458597 1 0.882897 -1.093057 -1.166673 1 0.954448 -2.076618 0.281122 1 2.542790 2.440658 2.233293 1 4.925050 1.835299 1.698428 1 5.411547 -0.132568 0.320527 1 -2.460127 3.091937 1.085846 1 -4.604204 2.610462 0.214204 1 -5.591318 0.479535 0.029280 1 -4.541179 -1.535611 -0.279278 1 -2.146445 -3.831650 -1.489931 1 -3.292569 -2.571001 -1.969065 1 -3.570796 -3.522995 -0.495095
18	Atomic Number X Y Z 6 -1.776281 1.305552 1.031836 7 -0.587919 1.889475 0.999986 6 0.319359 0.866493 0.894974 6 -0.206159 -0.369881 0.866504 6 -1.681467 -0.225843 1.004465

	6	1.764260	0.794987	0.819320
	7	2.055745	-0.546573	0.748969
	6	0.858738	-1.397277	0.770726
	6	2.746169	1.725531	0.809824
	6	4.078235	1.253748	0.723721
	6	4.364574	-0.069375	0.652756
	6	3.327657	-1.070405	0.661550
	6	-2.962057	2.020681	1.184841
	6	-4.253637	1.494684	1.085717
	6	-4.642864	0.310149	0.505168
	6	-3.859099	-0.672132	-0.173460
	6	-2.534583	-0.889273	-0.039287
	8	3.494083	-2.278349	0.601675
	8	-1.835327	-1.784014	-0.746026
	6	-2.469283	-2.504810	-1.783535
	1	-2.006391	-0.593032	1.982494
	1	0.807995	-1.996675	-0.131882
	1	0.902072	-2.078029	1.616631
	1	2.510023	2.770463	0.865575
	1	4.884130	1.968433	0.714532
	1	5.374921	-0.428856	0.587748
	1	-2.852187	3.069014	1.405764
	1	-5.051647	2.138869	1.417030
	1	-5.706720	0.144764	0.453736
	1	-4.406540	-1.304530	-0.849339
	1	-1.697437	-3.105681	-2.241728
	1	-2.893786	-1.827686	-2.517938
	1	-3.245576	-3.151422	-1.386348
17	Atomic Number	X	Y	Z
	6	-1.551700	0.279887	0.123093
	7	-0.608658	1.166980	-0.070291
	6	0.574304	0.465191	0.029592
	6	0.439738	-0.840752	0.291295
	6	-1.015430	-1.126484	0.411310
	6	1.975347	0.810594	-0.090932
	7	2.654107	-0.367754	0.116386
	6	1.764216	-1.504931	0.377513
	6	2.638909	1.962110	-0.343476
	6	4.052444	1.894302	-0.384245
	6	4.719835	0.731701	-0.181408
	6	4.025779	-0.501747	0.088624
	6	-2.931142	0.609309	0.168396

	6	-3.972250	-0.330394	0.190755
	6	-3.946726	-1.661773	-0.157021
	6	-2.857752	-2.439973	-0.662454
	6	-1.551017	-2.202148	-0.487607
	8	4.541333	-1.591359	0.282945
	8	-3.170274	1.927715	0.228150
	6	-4.476665	2.428777	0.047838
	1	-1.273299	-1.374258	1.446160
	1	1.929711	-2.281700	-0.364272
	1	1.986561	-1.933505	1.351048
	1	2.103480	2.877780	-0.503334
	1	4.610781	2.793951	-0.582399
	1	5.792514	0.680114	-0.212040
	1	-4.946976	0.056578	0.429190
	1	-4.902562	-2.159140	-0.143035
	1	-3.133779	-3.308869	-1.238636
	1	-0.832416	-2.846102	-0.965575
	1	-4.370783	3.501587	-0.027083
	1	-4.922396	2.042433	-0.863778
	1	-5.113351	2.194595	0.895996
20	Atomic Number	X	Y	Z
	6	1.611282	0.193370	-0.813974
	7	0.483904	1.119975	-0.894023
	6	-0.526464	0.436663	-0.491052
	6	-0.273184	-0.904000	-0.093749
	6	1.073627	-1.125347	-0.256603
	6	-1.952858	0.701370	-0.337303
	7	-2.504086	-0.464362	0.138342
	6	-1.537081	-1.559487	0.332995
	6	-2.709718	1.794334	-0.568326
	6	-4.097393	1.689308	-0.299674
	6	-4.641444	0.541861	0.169128
	6	-3.842821	-0.633793	0.420322
	6	2.781581	0.733793	-0.028587
	6	3.903530	0.014056	0.194884
	6	4.118677	-1.369641	-0.084706
	6	3.205764	-2.389742	-0.200213
	6	1.811291	-2.294307	-0.112117
	8	-4.255631	-1.701961	0.839893
	1	1.957829	0.019020	-1.835021
	1	-1.545886	-1.875014	1.371338
	1	-1.824559	-2.412416	-0.273797

	1	-2.262455	2.696137	-0.939443
	1	-4.729843	2.543488	-0.473180
	1	-5.692315	0.454747	0.375333
	8	2.614819	2.000905	0.342394
	1	4.748151	0.525271	0.620858
	1	5.154578	-1.668527	-0.085771
	1	3.612678	-3.385543	-0.266781
	1	1.262619	-3.204596	0.068676
	6	3.608511	2.636277	1.116854
	1	3.215993	3.613983	1.355763
	1	4.531102	2.744610	0.554196
	1	3.799947	2.082362	2.031069
TS10	Atomic Number	X	Y	Z
	6	1.533332	-0.266929	0.126164
	7	0.559458	-1.195444	0.047349
	6	-0.571781	-0.501399	0.007588
	6	-0.422070	0.862938	0.060485
	6	0.958961	1.108614	0.135578
	6	-1.987185	-0.829619	-0.019752
	7	-2.643033	0.378500	0.007845
	6	-1.745277	1.541602	0.070581
	6	-2.670048	-1.994516	-0.073634
	6	-4.083398	-1.913188	-0.103667
	6	-4.729592	-0.722269	-0.080395
	6	-4.013955	0.527074	-0.022285
	6	2.953224	-0.627834	0.017172
	6	3.990920	0.244483	-0.124860
	6	4.008507	1.655928	-0.190386
	6	2.966930	2.592717	-0.125928
	6	1.627336	2.388434	0.025008
	8	-4.512742	1.640912	0.004063
	1	1.327032	0.444227	1.229782
	1	-1.927697	2.188910	-0.781193
	1	-1.949946	2.112846	0.970538
	1	-2.148369	-2.931643	-0.094522
	1	-4.657088	-2.823821	-0.146523
	1	-5.801750	-0.657416	-0.101823
	8	3.107908	-1.955612	0.087214
	1	4.966408	-0.201572	-0.192433
	1	4.991275	2.077573	-0.314445
	1	3.275430	3.622443	-0.207264
	1	0.978031	3.245644	0.059304

	6	4.388350	-2.526587	-0.050113
	1	4.240016	-3.594968	0.009765
	1	5.049738	-2.208284	0.750915
	1	4.828679	-2.275401	-1.010794
TS11	Atomic Number	X	Y	Z
	6	-1.725266	1.275851	1.122513
	7	-0.518868	1.829346	1.400781
	6	0.371942	0.949547	0.966358
	6	-0.155669	-0.192164	0.401900
	6	-1.545210	-0.049143	0.474509
	6	1.821228	0.841573	0.997064
	7	2.110921	-0.378092	0.433809
	6	0.921690	-1.142965	0.024734
	6	2.802150	1.663502	1.431609
	6	4.135857	1.214007	1.276724
	6	4.422141	0.013714	0.716870
	6	3.385402	-0.872270	0.250710
	6	-2.946514	2.045873	1.248559
	6	-4.188739	1.674611	0.831199
	6	-4.613264	0.492225	0.198108
	6	-3.889359	-0.647036	-0.216209
	6	-2.558710	-0.917934	-0.110807
	8	3.553780	-1.967695	-0.260845
	8	-1.981348	-2.058954	-0.537553
	6	-2.756655	-3.035233	-1.198211
	1	-1.790664	0.150159	1.789295
	1	0.973892	-1.364751	-1.035353
	1	0.888354	-2.086739	0.558071
	1	2.563918	2.613168	1.870027
	1	4.941368	1.845008	1.613190
	1	5.432951	-0.330689	0.598899
	1	-2.812083	3.002639	1.720359
	1	-4.971557	2.393241	1.012472
	1	-5.666514	0.447904	-0.019864
	1	-4.492166	-1.406976	-0.680144
	1	-2.071375	-3.827546	-1.461937
	1	-3.207762	-2.630405	-2.099309
	1	-3.529670	-3.427878	-0.544229
2b	Atomic Number	X	Y	Z
	6	-1.435321	2.117931	-3.046111

	6	-0.594922	1.173623	-3.671718
	6	-0.011631	0.164478	-2.973330
	6	-0.245565	0.047945	-1.584447
	6	-1.088043	0.988090	-0.936483
	6	-1.679285	2.029963	-1.705132
	7	0.347505	-0.965929	-0.913380
	6	0.108377	-1.039418	0.360239
	6	-0.709217	-0.161497	1.099377
	6	-1.315968	0.864493	0.448925
	6	0.638887	-2.045548	1.278154
	7	0.140886	-1.757373	2.517849
	6	-0.728957	-0.582929	2.534435
	6	1.461642	-3.098770	1.077895
	6	1.782448	-3.887032	2.208773
	6	1.288529	-3.601297	3.438544
	6	0.410728	-2.480585	3.661776
	8	-0.079343	-2.149239	4.728728
	8	-2.462085	2.874008	-1.008584
	6	-3.089963	3.937652	-1.688094
	1	-1.874442	2.898305	-3.638003
	1	-0.419178	1.265705	-4.729649
	1	0.629661	-0.558090	-3.444363
	1	-1.952670	1.571810	0.948852
	1	-1.716010	-0.858323	2.891062
	1	-0.328227	0.165013	3.210673
	1	1.843365	-3.310429	0.098104
	1	2.435633	-4.734678	2.086572
	1	1.530132	-4.197700	4.299021
	1	-3.658109	4.475325	-0.942781
	1	-3.761552	3.567107	-2.457268
	1	-2.356306	4.603388	-2.133637
2b′	Atomic Number	X	Y	Z
	6	0.038541	0.000450	-0.071086
	6	-0.010123	0.000879	1.336835
	6	1.142060	0.000933	2.074040
	6	2.408899	0.000551	1.409795
	6	2.434488	0.000122	-0.009355
	6	1.223562	0.000080	-0.736411
	7	3.528998	0.000615	2.158298
	6	4.656791	0.000260	1.517515
	6	4.807956	-0.000185	0.115401
	6	3.691572	-0.000254	-0.654305

	6	5.988621	0.000251	2.117891
	7	6.889686	-0.000193	1.089831
	6	6.263047	-0.000500	-0.230650
	6	6.393498	0.000585	3.407455
	6	7.789060	0.000468	3.641992
	6	8.682782	0.000034	2.622277
	6	8.260916	-0.000350	1.244911
	8	8.990196	-0.000709	0.266495
	1	-0.888147	0.000421	-0.618408
	1	-0.968063	0.001163	1.821213
	1	3.735697	-0.000583	-1.730721
	1	6.574528	0.876075	-0.789127
	1	6.574274	-0.877502	-0.788598
	1	5.673140	0.000934	4.202315
	1	8.147941	0.000735	4.657535
	1	9.742834	-0.000046	2.796959
	1	1.256468	-0.000247	-1.812097
	8	1.190668	0.001327	3.411011
	6	-0.017446	0.001698	4.134150
	1	-0.605627	-0.886130	3.917635
	1	0.260722	0.001960	5.178197
	1	-0.605387	0.889561	3.917126
23	Atomic Number	X	Y	Z
	6	-1.704689	1.344165	0.919214
	7	-0.518890	1.881297	1.268841
	6	0.373877	0.964033	0.913045
	6	-0.155588	-0.179694	0.333591
	6	-1.526274	0.016729	0.312257
	6	1.814737	0.844316	0.976102
	7	2.112478	-0.381051	0.426808
	6	0.928117	-1.132074	-0.022868
	6	2.792343	1.659078	1.438533
	6	4.124159	1.195332	1.331429
	6	4.415934	-0.012815	0.789699
	6	3.385651	-0.890162	0.293636
	6	-2.885201	2.035299	1.145299
	6	-4.172982	1.636691	0.852128
	6	-4.590505	0.452527	0.262997
	6	-3.877706	-0.644369	-0.191799
	6	-2.504767	-0.859360	-0.178967
	8	3.562255	-1.990241	-0.207051
	8	-1.974151	-1.984947	-0.662272

	6	-2.780237	-3.011459	-1.209680
	1	1.009772	-1.341366	-1.083907
	1	0.878993	-2.082195	0.497837
	1	2.548865	2.612806	1.865089
	1	4.925092	1.819969	1.690191
	1	5.426415	-0.368256	0.706746
	1	-2.755670	3.000007	1.607838
	1	-4.955170	2.329417	1.111894
	1	-5.657321	0.365489	0.134022
	1	-4.479488	-1.429602	-0.609326
	1	-2.092059	-3.785434	-1.515264
	1	-3.331507	-2.655697	-2.073896
	1	-3.464381	-3.408335	-0.466866
22	Atomic Number	X	Y	Z
	6	1.807869	0.100391	0.026125
	7	0.727825	-0.640931	-0.217770
	6	-0.300029	0.185742	0.014078
	6	0.052513	1.455540	0.404911
	6	1.449468	1.471623	0.434883
	6	-1.741260	0.078496	-0.044301
	7	-2.219313	1.315608	0.321714
	6	-1.159590	2.287296	0.634986
	6	-2.587416	-0.928890	-0.364552
	6	-3.973189	-0.651904	-0.305608
	6	-4.442096	0.568142	0.055395
	6	-3.553723	1.649499	0.398849
	6	3.107025	-0.433725	-0.112251
	6	4.302409	0.248297	0.115749
	6	4.524521	1.552117	0.514529
	6	3.642009	2.582339	0.810609
	6	2.267268	2.540995	0.773381
	8	-3.890073	2.775251	0.733616
	8	3.113546	-1.702926	-0.496447
	6	4.316069	-2.419027	-0.691706
	1	-1.250542	3.145918	-0.022802
	1	-1.280694	2.637846	1.655102
	1	-2.205195	-1.890127	-0.648750
	1	-4.672313	-1.432710	-0.554624
	1	-5.494055	0.781521	0.101070
	1	5.198603	-0.321669	-0.040722
	1	5.567353	1.808628	0.610946
	1	4.088541	3.517582	1.101822

	1	1.755190	3.452304	1.040118
	1	4.011552	-3.409039	-0.996977
	1	4.918655	-1.969737	-1.474688
	1	4.888072	-2.485451	0.228312
TS24–$Sn(CH_3)_3$ (Triplet)	Atomic Number	X	Y	Z
	6	-3.601227	-1.884910	1.034026
	6	-3.236516	-1.106464	2.170218
	6	-2.000288	-0.558634	2.273196
	6	-1.074130	-0.671821	1.194670
	6	-1.329696	-1.689885	0.174664
	6	-2.687416	-2.169706	0.071080
	7	0.266290	-0.187740	1.450166
	6	1.196944	-0.755644	0.694841
	6	0.989257	-1.663683	-0.324986
	6	-0.323367	-2.124684	-0.643677
	6	2.625807	-0.479344	0.776432
	7	3.237332	-1.226373	-0.192036
	6	2.286837	-2.024093	-0.956071
	6	3.345989	0.331121	1.589119
	6	4.745182	0.362028	1.388091
	6	5.348883	-0.382405	0.427071
	6	4.593411	-1.246901	-0.441453
	8	5.044102	-1.953162	-1.330381
	8	-2.905741	-2.953027	-1.000776
	6	-4.169961	-3.555259	-1.152011
	1	-4.598774	-2.278067	0.975296
	1	-3.963009	-0.959721	2.949918
	1	-1.717463	0.048028	3.114931
	1	-0.506223	-2.830761	-1.429893
	1	2.336143	-1.764571	-2.010741
	1	2.525148	-3.081364	-0.872167
	1	2.859436	0.909738	2.350024
	1	5.348035	0.994886	2.018061
	1	6.412071	-0.359166	0.274740
	1	-4.118544	-4.139197	-2.059757
	1	-4.393643	-4.207973	-0.312618
	1	-4.951153	-2.806100	-1.248418
	1	-1.382764	0.475746	0.387509
	50	-1.019753	2.186289	-0.450003
	6	0.796596	2.106408	-1.568189
	1	1.647757	1.987169	-0.908372
	1	0.778412	1.281275	-2.271239

	1	0.915700	3.030086	-2.127090
	6	-2.690652	2.554160	-1.738715
	1	-3.618560	2.533782	-1.178527
	1	-2.585303	3.532121	-2.199491
	1	-2.739979	1.806455	-2.522125
	6	-0.942106	3.614273	1.134954
	1	-0.125982	3.383107	1.809161
	1	-0.788192	4.608596	0.726290
	1	-1.869715	3.612071	1.696243
TS25–$Sn(CH_3)_3$ (Triplet)	Atomic Number	X	Y	Z
	6	-2.890398	1.960320	2.098148
	6	-2.786743	2.673516	0.863748
	6	-1.703603	2.540280	0.059998
	6	-0.603476	1.660888	0.444293
	6	-0.880273	0.732158	1.562089
	6	-1.952482	1.056484	2.457553
	7	0.495931	1.686080	-0.232918
	6	1.516871	0.886145	0.233628
	6	1.438468	0.054595	1.382847
	6	0.287748	-0.040896	2.068907
	6	2.797126	0.781356	-0.325416
	7	3.539806	-0.093146	0.448230
	6	2.775477	-0.598581	1.584658
	6	3.364129	1.368861	-1.436512
	6	4.695069	1.042917	-1.733827
	6	5.414444	0.178560	-0.959573
	6	4.840825	-0.446841	0.211805
	8	5.420795	-1.225553	0.954356
	8	-1.499106	3.205028	-1.082159
	6	-2.462864	4.142545	-1.498192
	1	-3.731048	2.161032	2.738697
	1	-3.575416	3.353148	0.600114
	1	-2.036532	0.505569	3.378814
	1	0.163363	-0.655538	2.943452
	1	2.731604	-1.681880	1.555915
	1	3.253189	-0.309179	2.515064
	1	2.786601	2.047818	-2.033330
	1	5.162183	1.487899	-2.596530
	1	6.434457	-0.071915	-1.184528
	1	-2.094591	4.559426	-2.424478
	1	-2.578788	4.935987	-0.764438
	1	-3.424628	3.666957	-1.673018

	50	-1.815676	-1.805693	-0.453775
	1	-1.445123	-0.281784	0.747251
	6	-3.311624	-1.152777	-1.838522
	1	-4.209446	-0.844553	-1.314886
	1	-2.945951	-0.318075	-2.425569
	1	-3.564772	-1.966247	-2.512248
	6	-0.011021	-2.342771	-1.466200
	1	0.438955	-1.474017	-1.932653
	1	0.702778	-2.775706	-0.774546
	1	-0.232123	-3.074508	-2.237934
	6	-2.547046	-3.425711	0.741305
	1	-3.435714	-3.130004	1.287581
	1	-2.800594	-4.264785	0.099845
	1	-1.794392	-3.750785	1.450757
TS26–$Sn(CH_3)_3$ (Triplet)	Atomic Number	X	Y	Z
	6	-0.029078	-0.023072	0.023372
	7	0.001957	-0.009421	1.435110
	6	1.257150	-0.019978	1.722335
	6	2.131621	0.034296	0.589113
	6	1.338756	0.080270	-0.519933
	6	2.060776	-0.067378	2.925020
	7	3.373581	-0.034036	2.508423
	6	3.545951	0.029188	1.045301
	6	1.747128	-0.124480	4.240909
	6	2.819016	-0.147738	5.163896
	6	4.109799	-0.114296	4.752405
	6	4.461173	-0.052658	3.354050
	6	-1.231230	0.537295	-0.652864
	6	-1.356743	0.756705	-1.979937
	6	-0.405081	0.576000	-3.034564
	6	0.948807	0.287038	-2.986675
	6	1.757710	0.098700	-1.881801
	8	5.594899	-0.019530	2.904017
	1	-0.319777	-1.427796	-0.206718
	1	4.101623	0.923067	0.781564
	1	4.119690	-0.828106	0.707990
	1	0.720780	-0.146991	4.552620
	1	2.600671	-0.192850	6.217571
	1	4.928212	-0.131994	5.448245
	1	-2.313847	1.112050	-2.315873
	1	-0.811929	0.724837	-4.020760
	1	1.444144	0.240365	-3.943424

	1	2.813148	-0.030216	-2.054210
	50	-0.902086	-3.237917	-0.375410
	6	-0.756313	-3.852701	-2.419145
	6	-2.924623	-3.330072	0.310956
	6	0.382543	-4.411635	0.868809
	1	-1.333755	-3.195157	-3.058999
	1	-1.138856	-4.863689	-2.524726
	1	0.276115	-3.836605	-2.749415
	1	-3.582453	-2.796398	-0.365844
	1	-3.009651	-2.888479	1.297202
	1	-3.248918	-4.365223	0.363382
	1	1.409673	-4.351561	0.526729
	1	0.070316	-5.451481	0.839918
	1	0.337077	-4.065831	1.895249
	8	-2.214156	0.746041	0.229805
	6	-3.447247	1.271107	-0.202138
	1	-4.053068	1.369395	0.687074
	1	-3.317005	2.245822	-0.663488
	1	-3.936890	0.599374	-0.901956
TS27–$Sn(CH_3)_3$ (Triplet)	Atomic Number	X	Y	Z
	6	0.049820	-0.074724	0.035018
	7	0.073433	-0.033302	1.333377
	6	1.414344	-0.001983	1.669746
	6	2.242626	-0.030299	0.603362
	6	1.410267	-0.146167	-0.556858
	6	2.169634	0.050646	2.890208
	7	3.492133	0.044660	2.500242
	6	3.662176	-0.008267	1.042472
	6	1.836355	0.102244	4.205686
	6	2.896100	0.149293	5.138244
	6	4.197163	0.144421	4.749639
	6	4.568136	0.090807	3.359200
	6	-1.208693	-0.150523	-0.702936
	6	-1.356242	0.058842	-2.051854
	6	-0.411165	0.381917	-3.036400
	6	1.004284	0.504546	-2.956100
	6	1.818641	0.279429	-1.908288
	8	5.707630	0.081832	2.917560
	1	1.393414	-1.620544	-0.790520
	1	4.226097	0.857401	0.707752
	1	4.230010	-0.893775	0.769669
	1	0.806738	0.107252	4.506745

	1	2.662187	0.190378	6.189104
	1	5.002284	0.180280	5.459977
	1	-2.362815	-0.002108	-2.425303
	1	-0.826326	0.557082	-4.014096
	1	1.483562	0.810075	-3.872591
	1	2.878410	0.413454	-2.045537
	50	1.377619	-3.459438	-1.291948
	6	0.610671	-3.621602	-3.278335
	6	0.131471	-4.467890	0.119120
	6	3.401289	-4.138556	-1.176997
	1	-0.377953	-3.181999	-3.342533
	1	0.545162	-4.668575	-3.559349
	1	1.261496	-3.114025	-3.980936
	1	-0.882264	-4.086953	0.073864
	1	0.506502	-4.331653	1.126945
	1	0.114136	-5.530489	-0.104306
	1	4.037522	-3.574395	-1.849579
	1	3.448951	-5.186535	-1.457579
	1	3.783901	-4.036449	-0.167720
	8	-2.241684	-0.423480	0.109612
	6	-3.557463	-0.428174	-0.389331
	1	-4.192714	-0.636211	0.459686
	1	-3.822690	0.537492	-0.810577
	1	-3.694989	-1.203291	-1.138709
TS29–$Sn(CH_3)_3$ (Triplet)	Atomic Number	X	Y	Z
	6	0.141136	-0.300835	0.059554
	7	0.132787	-0.247544	1.461028
	6	1.372474	-0.057673	1.784003
	6	2.257757	0.104005	0.670056
	6	1.492304	0.003791	-0.443638
	6	2.139463	0.045348	3.003204
	7	3.444096	0.268713	2.618997
	6	3.643966	0.317604	1.157991
	6	1.800236	-0.026951	4.313861
	6	2.835320	0.136880	5.262822
	6	4.117835	0.357700	4.882583
	6	4.495720	0.437568	3.491867
	6	-1.115050	0.054691	-0.632361
	6	-1.257187	0.300587	-1.950210
	6	-0.278932	0.305602	-2.983749
	6	1.117249	0.176236	-2.918269
	6	1.927986	0.064114	-1.817717

	8	5.624907	0.632446	3.071322
	1	4.069115	1.274319	0.876205
	1	4.339922	-0.455625	0.853673
	1	0.780801	-0.199056	4.600684
	1	2.596011	0.084926	6.311678
	1	4.908896	0.482979	5.598773
	1	-1.979675	0.087750	0.007556
	1	-2.260412	0.515576	-2.282892
	1	-0.669793	0.449408	-3.976686
	1	1.610574	0.213080	-3.873089
	8	3.278179	0.021287	-1.893792
	6	3.922355	0.169771	-3.137923
	1	3.667464	-0.642181	-3.813333
	1	3.671051	1.120637	-3.599116
	1	4.982157	0.140129	-2.928510
	50	-0.121230	-3.587574	-0.515285
	6	1.825506	-4.372180	-0.930419
	1	2.504683	-4.170320	-0.109979
	1	1.762526	-5.447451	-1.070160
	1	2.230709	-3.929518	-1.833225
	6	-0.946332	-4.461722	1.251948
	1	-1.893330	-3.997304	1.501610
	1	-1.110889	-5.523433	1.093292
	1	-0.268890	-4.336429	2.088768
	6	-1.422433	-3.839843	-2.192345
	1	-1.446101	-4.886215	-2.482573
	1	-2.429463	-3.526290	-1.942183
	1	-1.076734	-3.253439	-3.035892
	1	0.105735	-1.698955	-0.161547
TS28–$Sn(CH_3)_3$ (Triplet)	Atomic Number	X	Y	Z
	6	0.023029	-0.000402	0.098512
	7	0.034280	0.116057	1.403618
	6	1.374696	0.095391	1.764714
	6	2.216318	-0.034945	0.721841
	6	1.385723	-0.182485	-0.447364
	6	2.110898	0.172117	2.996520
	7	3.436838	0.071842	2.634634
	6	3.625900	-0.064716	1.184382
	6	1.756585	0.312458	4.299807
	6	2.800543	0.350758	5.250670
	6	4.105846	0.252234	4.890065
	6	4.497967	0.103711	3.512534

	6	-1.208191	-0.040098	-0.626460
	6	-1.354533	-0.018884	-1.999832
	6	-0.394383	0.100085	-2.994606
	6	1.031483	0.227728	-2.908151
	6	1.822631	0.127320	-1.822609
	8	5.643250	0.007074	3.096789
	8	3.160175	0.258552	-1.844006
	6	3.816413	0.566206	-3.054874
	1	4.233983	0.751310	0.808944
	1	4.148621	-0.990366	0.962171
	1	0.723729	0.390939	4.578779
	1	2.550471	0.461264	6.292783
	1	4.899062	0.280309	5.614017
	1	-2.092719	-0.055173	-0.014101
	1	-2.371305	-0.069380	-2.355720
	1	-0.775731	0.130449	-4.001305
	1	1.515819	0.423982	-3.847511
	1	4.866711	0.639028	-2.812845
	1	3.467197	1.513412	-3.454267
	1	3.665549	-0.219174	-3.789717
	50	1.329448	-3.570089	-0.841783
	6	3.348509	-4.233278	-0.617880
	1	3.716995	-4.015103	0.378216
	1	3.401090	-5.306313	-0.775642
	1	3.994977	-3.747823	-1.340417
	6	0.057660	-4.390303	0.663585
	1	-0.953033	-4.014208	0.554972
	1	0.037371	-5.472273	0.573782
	1	0.418731	-4.132182	1.652501
	6	0.590039	-3.965826	-2.805208
	1	1.301754	-3.637986	-3.554313
	1	0.426576	-5.032551	-2.925793
	1	-0.348916	-3.450190	-2.970085
	1	1.352266	-1.705766	-0.581313
$\cdot Sn(CH_3)_3$	Atomic Number	X	Y	Z
	50	-0.928902	0.701476	0.419032
	6	-2.597484	-0.551442	-0.124330
	6	0.454445	-0.483334	1.572562
	6	0.063937	1.321867	-1.391504
	1	-2.236265	-1.403826	-0.693802
	1	-3.307622	-0.003484	-0.733551
	1	-3.108122	-0.916623	0.759762

	1	1.329162	0.098848	1.840248
	1	0.773542	-1.338564	0.982622
	1	-0.013355	-0.844544	2.481633
	1	0.932353	1.930323	-1.164899
	1	-0.607061	1.895744	-2.020907
	1	0.389571	0.442858	-1.941566

$HSn(CH_3)_3$	Atomic Number	X	Y	Z
	50	-0.860294	0.784627	0.290811
	6	-2.555343	-0.432456	-0.169364
	6	0.552863	-0.336847	1.436235
	6	0.049326	1.479645	-1.513772
	1	-1.374514	2.130721	1.207492
	1	-2.252035	-1.297654	-0.749890
	1	-3.284142	0.127563	-0.745822
	1	-3.034634	-0.781474	0.739209
	1	1.417090	0.271751	1.680832
	1	0.891734	-1.202300	0.876101
	1	0.106332	-0.682792	2.362542
	1	0.908383	2.104740	-1.293847
	1	-0.655388	2.061972	-2.098054
	1	0.382222	0.641003	-2.116673

CH_4	Atomic Number	X	Y	Z
	6	-0.627477	2.807133	0.000000
	1	-0.266096	1.784954	-0.000001
	1	-0.266076	3.318216	0.885230
	1	-0.266078	3.318217	-0.885230
	1	-1.711657	2.807147	0.000001