

“Core-first” approach for the Synthesis of Star-shaped polyisoprene with a Hyperbranched Core and isoprene catalyzed by half-sandwich scandium complexes

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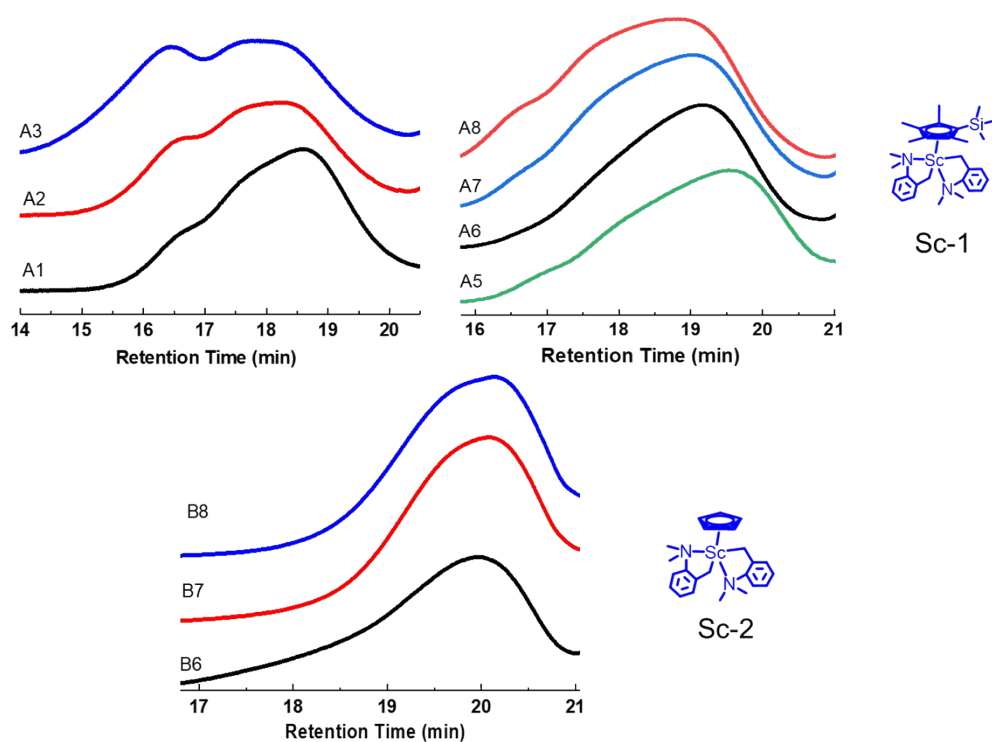


Figure S1 SEC curves of macromonomers (Runs A1-A3, A5-A8, B5-B8) given by refractive index detector

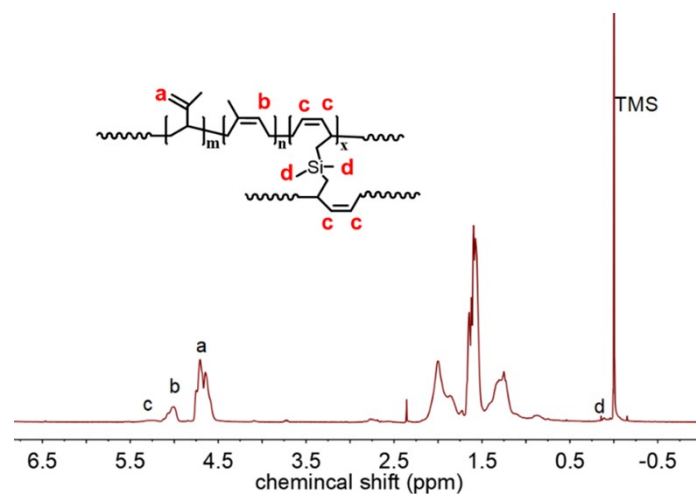


Figure S2 ^1H NMR spectrum of a typical Star-PIp (Run 2-2) in CDCl_3

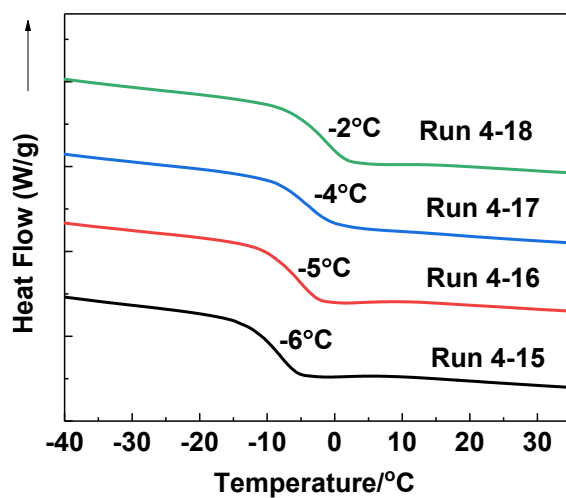
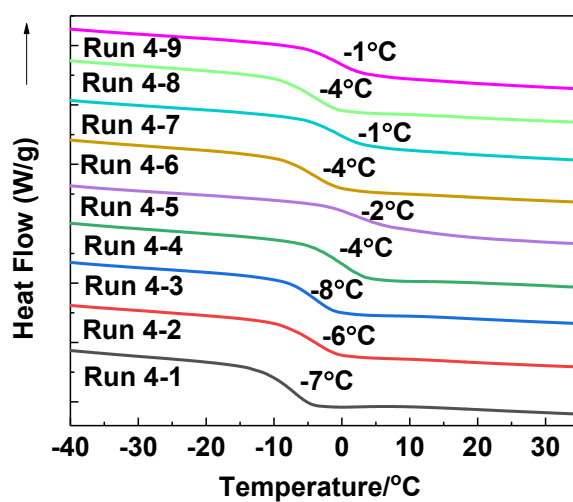


Figure S3 DSC curves of the other typical star-PIps

Table S1 Cartesian coordinates for important calculated structuresA [(C₅Me₄SiMe₃)Sc(CH₂C₆H₄NMe₂-*o*)]⁺

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	0.008701	0.227980	-0.365170
2	7	0	-1.343496	2.060575	-0.315684
3	6	0	-1.151460	-0.139673	-2.201611
4	1	0	-0.954059	0.722004	-2.849052
5	1	0	-1.165729	-1.056049	-2.791099
6	6	0	-2.297277	-0.016464	-1.282367
7	6	0	-2.384392	1.027379	-0.301687
8	6	0	-3.412389	1.036264	0.660700
9	1	0	-3.483098	1.848908	1.374272
10	6	0	-4.350756	0.016886	0.698137
11	1	0	-5.143088	0.037790	1.439486
12	6	0	-4.273423	-1.031666	-0.232847
13	1	0	-5.008349	-1.830926	-0.211554
14	6	0	-3.271469	-1.045210	-1.187307
15	1	0	-3.223531	-1.853336	-1.910557
16	6	0	-1.151291	2.776117	0.968886
17	1	0	-1.978898	3.462668	1.184717
18	1	0	-0.231270	3.363739	0.902585
19	1	0	-1.062932	2.064821	1.795428
20	6	0	-1.493464	3.046288	-1.419727
21	1	0	-1.690894	2.530763	-2.358131
22	1	0	-0.570209	3.625042	-1.513461
23	1	0	-2.329438	3.723776	-1.207089
24	6	0	1.304721	-1.821442	-0.251851
25	6	0	1.932784	-0.771593	0.509280
26	6	0	1.066959	-0.496219	1.633294
27	6	0	-0.083118	-1.326421	1.529282
28	6	0	0.069251	-2.147235	0.362350
29	6	0	1.321896	0.518463	2.723052
30	1	0	2.271338	0.314849	3.228078
31	1	0	0.535275	0.494309	3.481113
32	1	0	1.382755	1.549948	2.348944
33	6	0	-1.236986	-1.423005	2.492183
34	1	0	-2.196704	-1.469991	1.967381
35	1	0	-1.278743	-0.568361	3.173128
36	1	0	-1.154092	-2.327699	3.107102
37	6	0	-0.878657	-3.236309	-0.056346
38	1	0	-0.570254	-4.199829	0.369020
39	1	0	-0.914427	-3.351952	-1.143438
40	1	0	-1.895843	-3.035100	0.288211
41	6	0	1.835129	-2.456432	-1.513517
42	1	0	2.850739	-2.834873	-1.362547
43	1	0	1.210180	-3.297249	-1.822144
44	1	0	1.870988	-1.755118	-2.356778
45	14	0	3.265076	0.388622	-0.143226
46	6	0	4.477181	-0.417712	-1.333060
47	1	0	4.014372	-0.744223	-2.268636
48	1	0	5.268897	0.298479	-1.583812
49	1	0	4.955639	-1.289656	-0.872474
50	6	0	4.208206	1.309989	1.199841
51	1	0	4.649924	0.607735	1.916346
52	1	0	5.030241	1.874684	0.743876
53	1	0	3.591789	2.017477	1.762053
54	6	0	2.213757	1.676716	-1.136479
55	1	0	2.878361	2.412888	-1.604499
56	1	0	1.647890	1.251362	-1.987084
57	1	0	1.532632	2.288471	-0.517092

B [(C₅H₅)Sc(CH₂C₆H₄NMe₂-o)]⁺

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	-1.102328	0.727440	0.617972
2	7	0	1.001323	1.611463	-0.015969
3	6	0	0.326877	-0.116752	2.188733
4	1	0	0.815881	0.687059	2.739237
5	1	0	0.034148	-0.909745	2.877712
6	6	0	1.068289	-0.620272	1.028026
7	6	0	1.406935	0.214602	-0.075547
8	6	0	2.066393	-0.314433	-1.197968
9	1	0	2.349808	0.330731	-2.022111
10	6	0	2.369452	-1.664751	-1.265242
11	1	0	2.889815	-2.057979	-2.133473
12	6	0	2.007570	-2.514530	-0.209613
13	1	0	2.245014	-3.573466	-0.257255
14	6	0	1.364545	-2.000470	0.899853
15	1	0	1.104240	-2.655500	1.727372
16	6	0	0.946141	2.278495	-1.332779
17	1	0	1.948956	2.425092	-1.754388
18	1	0	0.483744	3.258997	-1.208816
19	1	0	0.348023	1.691655	-2.033307
20	6	0	1.877543	2.415086	0.868693
21	1	0	1.991150	1.940025	1.842023
22	1	0	1.450817	3.413798	0.998533
23	1	0	2.872763	2.515367	0.416475
24	6	0	-3.177018	0.316201	-0.735136
25	6	0	-2.047176	0.042962	-1.547711
26	6	0	-1.367755	-1.068342	-0.992755
27	6	0	-2.063376	-1.466773	0.179941
28	6	0	-3.190007	-0.622455	0.324447
29	1	0	-1.782849	0.565946	-2.460204
30	1	0	-3.920354	1.080338	-0.924498
31	1	0	-3.946636	-0.706527	1.094498
32	1	0	-1.798371	-2.295378	0.825130
33	1	0	-0.476984	-1.538315	-1.390218

SI (dimethyl-di-2,4-pentadienyl-(E,E)-silane)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	0.109312	1.240431	0.043823
2	6	0	-2.540198	0.213678	0.273624
3	6	0	-3.675235	-0.241740	-0.310201
4	1	0	-2.168594	-0.256682	1.159949
5	1	0	-4.046838	0.228619	-1.196527
6	6	0	-4.430220	-1.436227	0.302008
7	6	0	-5.565258	-1.891645	-0.281816
8	1	0	-4.058618	-1.906585	1.188335
9	1	0	-6.089825	-2.721580	0.143550
10	1	0	-5.936859	-1.421288	-1.168144
11	6	0	-1.785214	1.408166	-0.338584
12	1	0	-1.935564	1.420101	-1.397901
13	1	0	-2.155217	2.318681	0.084453
14	6	0	0.381909	1.218792	1.964454
15	1	0	0.011906	2.129307	2.387490
16	1	0	-0.142658	0.388856	2.389819
17	1	0	1.426828	1.126279	2.175369
18	6	0	1.060395	2.745175	-0.727400
19	1	0	0.910046	2.757110	-1.786717
20	1	0	0.690392	3.655690	-0.304363
21	1	0	2.105314	2.652662	-0.516485
22	6	0	0.780158	-0.410410	-0.723178
23	6	0	1.958746	-1.145363	-0.058065

24	1	0	-0.039479	-1.097147	-0.761721
25	6	0	3.231087	-0.856296	-0.424335
26	1	0	1.773055	-1.884246	0.693248
27	1	0	3.416778	-0.117412	-1.175646
28	6	0	4.409675	-1.591250	0.240779
29	6	0	5.682016	-1.302183	-0.125491
30	1	0	4.223984	-2.330133	0.992091
31	1	0	6.500905	-1.812834	0.336630
32	1	0	5.867707	-0.563300	-0.876805
33	1	0	1.069208	-0.196318	-1.730906

SIATS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	0.963223	-0.392865	-0.300338
2	7	0	0.756803	-2.760806	0.033750
3	6	0	2.537622	-1.423175	-1.892081
4	1	0	2.361991	-2.238627	-2.592527
5	1	0	3.298344	-0.760985	-2.307150
6	6	0	2.984868	-1.908129	-0.557399
7	6	0	2.156619	-2.612461	0.360230
8	6	0	2.689174	-3.085489	1.572603
9	1	0	2.063624	-3.645787	2.258559
10	6	0	4.017045	-2.861629	1.898574
11	1	0	4.415428	-3.253096	2.829976
12	6	0	4.838407	-2.133748	1.027525
13	1	0	5.879424	-1.953315	1.278855
14	6	0	4.321557	-1.656486	-0.162539
15	1	0	4.964163	-1.109497	-0.847717
16	6	0	-0.117178	-3.066722	1.181709
17	1	0	0.031346	-4.092295	1.545489
18	1	0	-1.155086	-2.966545	0.858067
19	1	0	0.065327	-2.367035	1.999836
20	6	0	0.504815	-3.768383	-1.020211
21	1	0	1.122795	-3.584617	-1.897324
22	1	0	-0.548307	-3.733847	-1.311373
23	1	0	0.731349	-4.773813	-0.641916
24	6	0	2.583597	0.907532	1.045615
25	6	0	1.821610	1.836037	0.291128
26	6	0	0.481465	1.768443	0.738353
27	6	0	0.408233	0.783596	1.756131
28	6	0	1.712770	0.265506	1.957852
29	6	0	0.890829	-0.504718	-2.813286
30	6	0	0.192805	0.589045	-2.245595
31	1	0	0.336925	-1.428034	-2.977532
32	1	0	1.575730	-0.276813	-3.623100
33	6	0	-1.029234	0.472253	-1.498689
34	6	0	-1.609863	-0.686231	-1.047414
35	1	0	-1.465908	1.411924	-1.163724
36	1	0	-1.264196	-1.635547	-1.462201
37	1	0	0.564591	1.588580	-2.446978
38	6	0	-2.875160	-0.731510	-0.259368
39	14	0	-4.465102	-0.977617	-1.337576
40	1	0	-3.029484	0.198264	0.302539
41	1	0	-2.867914	-1.549140	0.474121
42	6	0	-4.553905	0.386075	-2.643838
43	6	0	-4.414528	-2.686987	-2.156237
44	6	0	-5.941830	-0.864294	-0.123462
45	1	0	-5.471424	0.290524	-3.236236
46	1	0	-4.556434	1.382656	-2.188178
47	1	0	-3.707827	0.333682	-3.338340
48	1	0	-4.328706	-3.490098	-1.414653
49	1	0	-5.333118	-2.866388	-2.726863
50	1	0	-3.576687	-2.776314	-2.858378
51	6	0	-6.033684	0.475541	0.530785
52	1	0	-5.836008	-1.661639	0.624398

53	1	0	-6.854969	-1.083729	-0.695001
54	6	0	-5.664863	0.758150	1.794743
55	1	0	-6.411670	1.290461	-0.089440
56	1	0	-5.303762	-0.047185	2.438283
57	6	0	-5.732269	2.082116	2.388767
58	6	0	-5.369128	2.368378	3.647832
59	1	0	-6.111713	2.880864	1.750085
60	1	0	-5.445481	3.374463	4.048957
61	1	0	-4.996832	1.600138	4.322989
62	14	0	2.587374	3.207772	-0.847093
63	6	0	4.105836	4.017700	0.048389
64	1	0	4.850955	3.272055	0.231997
65	1	0	4.516483	4.787280	-0.571301
66	1	0	3.787574	4.440478	0.978371
67	6	0	1.251146	4.566332	-1.210982
68	1	0	1.634767	5.260609	-1.929114
69	1	0	0.368096	4.103166	-1.599056
70	1	0	1.013585	5.084527	-0.305479
71	6	0	3.170902	2.411022	-2.516908
72	1	0	2.358313	1.872848	-2.958462
73	1	0	3.494006	3.181121	-3.185827
74	1	0	3.982231	1.739650	-2.327417
75	6	0	-0.694079	2.609933	0.207702
76	1	0	-0.440741	3.648292	0.258001
77	1	0	-0.895474	2.340740	-0.808111
78	1	0	-1.562800	2.425438	0.804517
79	6	0	-0.855989	0.387726	2.541389
80	1	0	-1.230336	1.240556	3.068119
81	1	0	-1.601873	0.032948	1.861176
82	1	0	-0.614145	-0.385381	3.240473
83	6	0	2.117518	-0.786236	3.007430
84	1	0	1.893274	-0.417635	3.986587
85	1	0	1.573566	-1.691140	2.833747
86	1	0	3.166937	-0.980691	2.931211
87	6	0	4.099866	0.672216	0.914643
88	1	0	4.306825	0.190853	-0.018286
89	1	0	4.611143	1.611397	0.952545
90	1	0	4.435141	0.050902	1.718670

2SIA TS²

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	-0.591051	1.240197	0.033235
2	6	0	-1.988019	-0.694741	1.393428
3	1	0	-1.157864	-1.393909	1.519017
4	6	0	-2.314894	-0.487115	0.000762
5	6	0	-1.475368	-0.707588	-1.069069
6	1	0	-1.871847	-0.533529	-2.065252
7	6	0	-0.117515	3.609902	-0.466100
8	6	0	-1.541064	3.406945	-0.536630
9	6	0	-1.776056	2.550642	-1.667238
10	6	0	-0.525663	2.200305	-2.246724
11	6	0	0.502611	2.844202	-1.493671
12	1	0	-3.299834	-0.075202	-0.219328
13	6	0	-1.130631	0.788172	2.574218
14	6	0	-0.236111	1.835762	2.196906
15	1	0	-0.695213	-0.039220	3.133802
16	1	0	-2.071277	1.133434	2.992355
17	6	0	1.113122	1.608918	1.771362
18	6	0	1.620168	0.389075	1.383716
19	1	0	1.738123	2.487562	1.623956
20	1	0	1.040129	-0.506086	1.626652
21	1	0	-0.568974	2.860921	2.322505
22	6	0	-0.108397	-1.315179	-0.975250
23	6	0	0.332349	-2.038171	-2.261946
24	1	0	0.685735	-0.554149	-0.736559
25	1	0	-0.044456	-2.028562	-0.143668

26	1	0	-0.405459	-2.821462	-2.460664
27	1	0	0.285762	-1.342835	-3.106823
28	6	0	1.731271	-2.598568	-2.148948
29	6	0	2.013640	-3.742500	-1.367928
30	6	0	2.788707	-1.932281	-2.775162
31	7	0	0.929270	-4.449836	-0.762438
32	6	0	3.345620	-4.144211	-1.207281
33	6	0	4.111471	-2.346033	-2.620928
34	1	0	2.569265	-1.066763	-3.398194
35	6	0	1.240273	-5.129198	0.487383
36	6	0	0.259458	-5.367512	-1.686462
37	1	0	3.573261	-5.022799	-0.611208
38	6	0	4.388289	-3.450082	-1.820304
39	1	0	4.913237	-1.813216	-3.124496
40	1	0	1.856545	-6.036247	0.360515
41	1	0	0.302244	-5.436108	0.962599
42	1	0	1.762890	-4.447403	1.164697
43	1	0	0.034040	-4.868666	-2.632106
44	1	0	-0.681200	-5.711247	-1.241918
45	1	0	0.878210	-6.252231	-1.914034
46	1	0	5.411910	-3.791164	-1.689195
47	6	0	-3.153736	-0.996422	2.313917
48	14	0	-3.944989	-2.757065	2.186699
49	1	0	-3.949725	-0.251160	2.176608
50	6	0	-2.596421	-4.043512	1.842946
51	6	0	-4.756068	-3.088754	3.865559
52	6	0	-5.324108	-2.861669	0.857460
53	1	0	-3.030476	-5.049876	1.810825
54	1	0	-2.086920	-3.869127	0.888287
55	1	0	-1.839818	-4.040956	2.636928
56	1	0	-5.516740	-2.335209	4.100932
57	1	0	-5.248138	-4.068148	3.875166
58	1	0	-4.017144	-3.082263	4.675352
59	6	0	-4.893573	-2.817824	-0.569504
60	1	0	-6.071212	-2.083885	1.065025
61	1	0	-5.819503	-3.824575	1.062735
62	6	0	-5.270128	-1.898687	-1.478736
63	1	0	-4.226417	-3.617859	-0.897483
64	1	0	-5.960163	-1.105376	-1.183525
65	6	0	-4.833526	-1.903587	-2.864497
66	6	0	-5.202426	-1.000834	-3.787820
67	1	0	-4.172109	-2.720646	-3.158006
68	1	0	-4.865467	-1.068044	-4.818061
69	1	0	-5.881516	-0.185002	-3.547861
70	1	0	-2.836115	-0.913680	3.362642
71	6	0	3.019879	0.157627	0.927438
72	14	0	4.237935	-0.350533	2.339155
73	1	0	3.444094	1.062021	0.473823
74	1	0	3.067429	-0.637375	0.171631
75	6	0	4.200406	0.949926	3.712445
76	6	0	3.758117	-2.055178	3.013569
77	6	0	5.970675	-0.433556	1.523923
78	1	0	4.918157	0.698617	4.502185
79	1	0	4.461210	1.944063	3.331938
80	1	0	3.210007	1.015814	4.177004
81	1	0	3.767293	-2.810209	2.218906
82	1	0	4.462926	-2.379224	3.788032
83	1	0	2.759111	-2.045662	3.466019
84	6	0	6.430078	0.897886	1.028936
85	1	0	5.921490	-1.163282	0.704892
86	1	0	6.669432	-0.834494	2.271817
87	6	0	6.420472	1.302727	-0.255541
88	1	0	6.776624	1.601989	1.787836
89	1	0	6.092571	0.606625	-1.030496
90	6	0	6.839698	2.620786	-0.699014
91	6	0	6.837573	3.030423	-1.976493
92	1	0	7.181262	3.306638	0.077600
93	1	0	7.169683	4.025271	-2.257600
94	1	0	6.517462	2.375539	-2.784785

95	6	0	0.611794	4.604906	0.390184
96	1	0	0.446651	5.620289	0.007861
97	1	0	0.289496	4.606545	1.434982
98	1	0	1.692917	4.439678	0.370237
99	6	0	1.963251	2.827290	-1.844792
100	1	0	2.603781	3.044318	-0.985548
101	1	0	2.279233	1.859934	-2.249388
102	1	0	2.186627	3.582697	-2.610014
103	6	0	-0.323707	1.490139	-3.552857
104	1	0	0.629316	0.953119	-3.592682
105	1	0	-1.125142	0.778710	-3.774310
106	1	0	-0.310439	2.216281	-4.377120
107	6	0	-3.110347	2.203778	-2.263110
108	1	0	-3.359743	2.913124	-3.063622
109	1	0	-3.133507	1.205846	-2.713117
110	1	0	-3.919187	2.252946	-1.530127
111	14	0	-2.926764	4.347618	0.390223
112	6	0	-3.815216	5.456630	-0.863547
113	1	0	-4.300171	4.884987	-1.661395
114	1	0	-4.589820	6.048186	-0.360937
115	1	0	-3.113406	6.156028	-1.332022
116	6	0	-2.284123	5.456206	1.788318
117	1	0	-1.788621	4.905353	2.595794
118	1	0	-1.601668	6.234515	1.433803
119	1	0	-3.150047	5.962483	2.233247
120	6	0	-4.180528	3.156888	1.187849
121	1	0	-3.710245	2.524055	1.949898
122	1	0	-4.957590	3.743829	1.693107
123	1	0	-4.688092	2.504257	0.469794

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	2.405736	-0.205671	-0.673416
2	6	0	0.409241	-1.411559	-2.141075
3	1	0	-0.259569	-0.550905	-2.201851
4	6	0	0.609285	-1.875186	-0.786065
5	6	0	0.432593	-1.153685	0.375327
6	1	0	0.642313	-1.663496	1.309795
7	6	0	4.800438	0.127217	-0.169705
8	6	0	4.504412	-1.280212	-0.116722
9	6	0	3.641366	-1.473619	1.019253
10	6	0	3.369844	-0.209691	1.610662
11	6	0	4.075782	0.782964	0.865472
12	1	0	1.003562	-2.888018	-0.681143
13	6	0	1.958316	-0.483464	-3.250107
14	6	0	3.024350	0.343338	-2.790256
15	1	0	1.134558	0.016216	-3.758427
16	1	0	2.272640	-1.399354	-3.741192
17	6	0	2.819200	1.653794	-2.241317
18	6	0	1.605418	2.124330	-1.800070
19	1	0	3.705477	2.253097	-2.042429
20	1	0	0.711573	1.565454	-2.090988
21	1	0	4.041935	0.002407	-2.948441
22	6	0	-0.172846	0.216682	0.479452
23	1	0	0.570066	0.950772	0.858485
24	1	0	-0.497779	0.583636	-0.498809
25	6	0	0.096168	-2.474120	-3.173878
26	14	0	-1.679786	-3.254029	-3.115340
27	1	0	0.817896	-3.298301	-3.091616
28	6	0	-2.813858	-2.319931	-1.920831
29	6	0	-2.394132	-3.191261	-4.867716
30	6	0	-1.532057	-5.091696	-2.585989
31	1	0	-3.812487	-2.772196	-1.920308
32	1	0	-2.437229	-2.341024	-0.892337
33	1	0	-2.937487	-1.272372	-2.219148
34	1	0	-1.746732	-3.709930	-5.584424

35	1	0	-3.379921	-3.668904	-4.905580
36	1	0	-2.515545	-2.157294	-5.211989
37	6	0	-0.941626	-5.303549	-1.234043
38	1	0	-0.948785	-5.618974	-3.352625
39	1	0	-2.551727	-5.503420	-2.626350
40	6	0	0.265185	-5.847376	-0.981407
41	1	0	-1.550795	-4.988226	-0.383999
42	1	0	0.878320	-6.195776	-1.814783
43	6	0	0.805194	-6.045146	0.352820
44	6	0	1.990661	-6.616681	0.620588
45	1	0	0.176101	-5.717178	1.182295
46	1	0	2.335381	-6.764228	1.639742
47	1	0	2.638710	-6.983279	-0.172970
48	1	0	0.204523	-2.062468	-4.185887
49	6	0	1.361362	3.470506	-1.209056
50	14	0	0.891036	4.814534	-2.517237
51	1	0	2.248042	3.848705	-0.685899
52	1	0	0.541556	3.435098	-0.479646
53	6	0	2.295680	4.983499	-3.772815
54	6	0	-0.723534	4.328875	-3.383093
55	6	0	0.646535	6.448094	-1.545028
56	1	0	2.060910	5.756937	-4.513518
57	1	0	3.238017	5.263732	-3.288490
58	1	0	2.461098	4.046852	-4.317302
59	1	0	-1.539582	4.190858	-2.664265
60	1	0	-1.032617	5.108743	-4.088729
61	1	0	-0.611611	3.399464	-3.954259
62	6	0	1.891317	6.895563	-0.852301
63	1	0	-0.171056	6.300171	-0.826862
64	1	0	0.306321	7.207457	-2.263846
65	6	0	2.131122	6.798391	0.469187
66	1	0	2.673439	7.315381	-1.487821
67	1	0	1.353565	6.399138	1.124104
68	6	0	3.368060	7.213264	1.107605
69	6	0	3.611095	7.124385	2.423822
70	1	0	4.135602	7.627852	0.452519
71	1	0	4.550812	7.456828	2.854466
72	1	0	2.869461	6.728629	3.115173
73	6	0	5.847133	0.802667	-1.007951
74	1	0	6.844063	0.594210	-0.598533
75	1	0	5.860751	0.471380	-2.049019
76	1	0	5.732731	1.890569	-1.001647
77	6	0	4.160429	2.235345	1.238631
78	1	0	4.418817	2.872501	0.388111
79	1	0	3.220004	2.611231	1.654731
80	1	0	4.932489	2.393472	2.003433
81	6	0	2.649518	0.036335	2.902823
82	1	0	2.188306	1.028873	2.937887
83	1	0	1.865698	-0.699366	3.100087
84	1	0	3.346443	-0.015794	3.749448
85	6	0	3.227494	-2.791801	1.607125
86	1	0	4.025951	-3.179075	2.253559
87	1	0	2.338192	-2.701683	2.238565
88	1	0	3.024946	-3.559031	0.854903
89	14	0	5.324091	-2.708638	-1.091161
90	6	0	6.365651	-3.736906	0.112743
91	1	0	5.756834	-4.234187	0.874518
92	1	0	6.909683	-4.515488	-0.435500
93	1	0	7.105465	-3.112826	0.626772
94	6	0	6.469261	-2.112002	-2.480587
95	1	0	5.950605	-1.546990	-3.263596
96	1	0	7.304616	-1.507180	-2.114867
97	1	0	6.897956	-3.000952	-2.960274
98	6	0	4.018969	-3.822189	-1.913228
99	1	0	3.392027	-3.258444	-2.614835
100	1	0	4.527991	-4.602296	-2.493134
101	1	0	3.362650	-4.328583	-1.197845
102	6	0	-1.424749	0.328444	1.424799
103	6	0	-1.153793	-0.140009	2.860706

104	14	0	-2.632842	-0.190823	4.085499
105	1	0	-0.372785	0.482978	3.318939
106	1	0	-0.755198	-1.164443	2.856826
107	6	0	-3.185406	1.537444	4.628665
108	6	0	-4.081222	-1.156495	3.335557
109	6	0	-2.001528	-1.156995	5.622688
110	1	0	-3.951640	1.462950	5.409697
111	1	0	-2.350942	2.118830	5.037694
112	1	0	-3.611289	2.102457	3.793646
113	1	0	-3.766839	-2.155279	3.009230
114	1	0	-4.869844	-1.291043	4.085776
115	1	0	-4.529470	-0.644260	2.476130
116	6	0	-0.784501	-0.560610	6.245139
117	1	0	-1.817042	-2.198955	5.328201
118	1	0	-2.832863	-1.173221	6.343436
119	6	0	0.447285	-1.105253	6.242876
120	1	0	-0.914624	0.409170	6.730433
121	1	0	0.594683	-2.086885	5.787227
122	6	0	1.615510	-0.482569	6.840163
123	6	0	2.842064	-1.027109	6.869357
124	1	0	1.459073	0.493754	7.301466
125	1	0	3.678682	-0.524109	7.345113
126	1	0	3.040938	-2.006929	6.439013
127	6	0	-1.883860	1.764616	1.392858
128	6	0	-2.871154	2.300703	0.661336
129	1	0	-1.312407	2.433150	2.040926
130	1	0	-3.040607	3.373860	0.772885
131	6	0	-3.804021	1.618103	-0.294637
132	6	0	-5.284731	1.941088	-0.001403
133	1	0	-3.575115	1.950179	-1.318878
134	1	0	-3.669172	0.530771	-0.285340
135	1	0	-5.519264	1.589769	1.005637
136	1	0	-5.418347	3.031750	-0.005604
137	6	0	-6.207100	1.306968	-1.016994
138	6	0	-6.978421	0.162138	-0.719904
139	6	0	-6.250237	1.826728	-2.314664
140	7	0	-6.976535	-0.353409	0.612757
141	6	0	-7.727619	-0.438515	-1.740980
142	6	0	-7.002518	1.228665	-3.322861
143	1	0	-5.671005	2.721288	-2.539849
144	6	0	-7.178089	-1.787210	0.735877
145	6	0	-7.870194	0.376051	1.510380
146	1	0	-8.326107	-1.317508	-1.520349
147	6	0	-7.734256	0.080296	-3.033628
148	1	0	-7.016178	1.655684	-4.322070
149	1	0	-8.217124	-2.112494	0.547265
150	1	0	-6.920188	-2.092322	1.756281
151	1	0	-6.518465	-2.316200	0.041631
152	1	0	-7.697861	1.452420	1.429481
153	1	0	-7.675913	0.071646	2.545261
154	1	0	-8.934953	0.186408	1.287455
155	1	0	-8.327976	-0.402987	-3.805423
156	1	0	-2.191961	-0.314471	0.976601

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	-5.710965	-0.796555	0.396694
2	6	0	-7.046893	1.249113	-1.712703
3	1	0	-6.153212	1.869640	-1.568962
4	6	0	-7.655546	0.910321	-0.382937
5	6	0	-7.212921	1.198934	0.863417
6	1	0	-7.854666	0.905035	1.693030
7	6	0	-4.628891	-2.683877	1.461122
8	6	0	-5.962717	-3.064881	1.072871
9	6	0	-6.858396	-2.283968	1.890994
10	6	0	-6.091277	-1.440288	2.742482

11	6	0	-4.708940	-1.675526	2.461779
12	1	0	-8.605053	0.373604	-0.441997
13	6	0	-6.656969	-0.045909	-2.491285
14	6	0	-5.771770	-1.144242	-1.883578
15	1	0	-6.199572	0.294572	-3.432615
16	1	0	-7.599550	-0.529955	-2.775244
17	6	0	-4.385158	-1.012543	-1.598825
18	6	0	-3.775270	0.050007	-0.943769
19	1	0	-3.795809	-1.930915	-1.657099
20	1	0	-4.295329	1.016100	-0.958687
21	1	0	-6.041651	-2.128136	-2.262499
22	6	0	-5.970365	1.964411	1.239078
23	1	0	-5.184873	1.330996	1.699790
24	1	0	-5.521332	2.506568	0.404006
25	6	0	-8.055880	2.043791	-2.576649
26	14	0	-8.640716	3.823828	-2.115001
27	1	0	-8.953731	1.425590	-2.726557
28	6	0	-7.288565	4.771695	-1.180951
29	6	0	-9.012800	4.684676	-3.758415
30	6	0	-10.271066	3.800165	-1.099378
31	1	0	-7.584386	5.819686	-1.053969
32	1	0	-7.104733	4.363162	-0.181114
33	1	0	-6.341919	4.769195	-1.734794
34	1	0	-9.769567	4.140065	-4.334956
35	1	0	-9.393178	5.698863	-3.591419
36	1	0	-8.114173	4.766746	-4.381035
37	6	0	-10.159482	3.390254	0.328296
38	1	0	-10.994652	3.170115	-1.633677
39	1	0	-10.653921	4.830484	-1.159665
40	6	0	-10.674081	2.272325	0.876242
41	1	0	-9.614904	4.074692	0.982803
42	1	0	-11.250178	1.585032	0.253302
43	6	0	-10.531050	1.923204	2.279248
44	6	0	-11.003983	0.799855	2.846214
45	1	0	-10.016024	2.653797	2.906316
46	1	0	-10.900726	0.611953	3.911029
47	1	0	-11.558467	0.060853	2.270903
48	1	0	-7.608081	2.140643	-3.576562
49	6	0	-2.301456	0.129413	-0.645192
50	14	0	-1.335612	1.019378	-2.059617
51	1	0	-1.883061	-0.878749	-0.524458
52	1	0	-2.114831	0.671327	0.292520
53	6	0	-1.511157	0.018819	-3.653438
54	6	0	-2.024042	2.770705	-2.280820
55	1	0	-1.008267	0.519613	-4.489109
56	1	0	-1.083241	-0.985264	-3.555116
57	1	0	-2.565168	-0.094269	-3.931028
58	1	0	-1.964046	3.352088	-1.353046
59	1	0	-1.462144	3.315980	-3.047975
60	1	0	-3.071528	2.752362	-2.603506
61	6	0	-3.343162	-3.311491	1.005826
62	1	0	-3.149510	-4.230724	1.574953
63	1	0	-3.358852	-3.587469	-0.050384
64	1	0	-2.488830	-2.648059	1.172390
65	6	0	-3.554924	-1.062484	3.204267
66	1	0	-2.664140	-0.958876	2.576321
67	1	0	-3.799290	-0.072158	3.603382
68	1	0	-3.274162	-1.686990	4.062821
69	6	0	-6.610494	-0.566182	3.848027
70	1	0	-6.027603	0.353570	3.970827
71	1	0	-7.657404	-0.283829	3.705980
72	1	0	-6.555606	-1.101479	4.804992
73	6	0	-8.359552	-2.378773	1.900403
74	1	0	-8.684192	-3.298734	2.403572
75	1	0	-8.821719	-1.544180	2.435084
76	1	0	-8.784420	-2.403530	0.892492
77	14	0	-6.487530	-4.590386	0.031005
78	6	0	-6.749756	-6.011336	1.255042
79	1	0	-7.528150	-5.776160	1.989463

80	1	0	-7.058178	-6.920230	0.724896
81	1	0	-5.830615	-6.241592	1.805568
82	6	0	-5.168946	-5.113128	-1.230932
83	1	0	-4.865313	-4.305552	-1.907240
84	1	0	-4.272451	-5.528570	-0.760239
85	1	0	-5.598754	-5.907019	-1.854274
86	6	0	-8.096414	-4.285390	-0.931253
87	1	0	-8.096107	-3.335217	-1.478047
88	1	0	-8.214799	-5.085198	-1.672471
89	1	0	-8.982827	-4.313384	-0.290051
90	6	0	0.536609	1.211205	-1.619542
91	6	0	1.309906	-0.057216	-1.429674
92	6	0	1.786367	-0.853203	-2.444065
93	1	0	1.321607	-0.462196	-0.414783
94	6	0	2.569976	-2.039887	-2.252165
95	1	0	1.680822	-0.497271	-3.467196
96	21	0	4.041229	-0.482064	-1.478867
97	6	0	2.705543	-2.692360	-0.993615
98	1	0	3.016131	-2.507104	-3.123473
99	1	0	1.827626	-2.712836	-0.349183
100	1	0	3.236598	-3.638709	-1.024118
101	1	0	3.328940	2.843327	-3.098310
102	6	0	3.616325	2.130212	-3.878464
103	6	0	4.528879	1.057330	-3.356634
104	1	0	2.698068	1.723008	-4.312711
105	1	0	4.113385	2.708345	-4.668781
106	6	0	4.651866	-0.270031	-3.858012
107	6	0	5.554785	1.262653	-2.384733
108	6	0	5.721162	-0.928634	-3.155035
109	6	0	3.918311	-0.773908	-5.067340
110	6	0	6.293549	0.053246	-2.270735
111	6	0	5.909809	2.583911	-1.770533
112	14	0	6.520051	-2.634015	-3.519352
113	1	0	4.565160	-0.700113	-5.950986
114	1	0	3.609685	-1.819407	-4.993589
115	1	0	3.030536	-0.172912	-5.286098
116	6	0	7.565211	-0.090871	-1.486238
117	1	0	5.036638	3.233268	-1.647714
118	1	0	6.390084	2.485916	-0.793826
119	1	0	6.618794	3.125928	-2.409672
120	6	0	8.255554	-2.341050	-4.216178
121	6	0	5.547936	-3.660572	-4.783212
122	6	0	6.627431	-3.688239	-1.939863
123	1	0	8.425680	0.118626	-2.134907
124	1	0	7.625325	0.622698	-0.658837
125	1	0	7.711908	-1.092954	-1.075007
126	1	0	8.926709	-1.870953	-3.490542
127	1	0	8.704694	-3.297546	-4.509309
128	1	0	8.221275	-1.703431	-5.106754
129	1	0	4.536144	-3.923217	-4.452988
130	1	0	5.477806	-3.178372	-5.762955
131	1	0	6.089668	-4.604017	-4.926317
132	1	0	5.636574	-3.870904	-1.505760
133	1	0	7.050390	-4.668053	-2.194680
134	1	0	7.267399	-3.253680	-1.165010
135	6	0	3.686513	-2.021509	0.781030
136	1	0	2.803700	-1.505296	1.162981
137	6	0	4.859052	-1.177759	0.732309
138	6	0	3.873535	-3.398219	1.379826
139	6	0	4.889477	0.199289	0.687333
140	1	0	5.818092	-1.695057	0.663661
141	14	0	4.102401	-3.487682	3.307275
142	1	0	4.747274	-3.886791	0.927707
143	1	0	3.006714	-4.033067	1.154001
144	1	0	5.864327	0.673519	0.646719
145	6	0	3.705505	1.108505	0.845863
146	6	0	3.729774	-1.816508	4.121030
147	6	0	2.906770	-4.801929	3.962916
148	6	0	5.894497	-4.034743	3.698439

149	1	0	3.534022	1.702010	-0.078170
150	1	0	2.787695	0.539580	1.025288
151	6	0	3.817480	2.149221	2.019748
152	1	0	3.840002	-1.896306	5.208865
153	1	0	4.409852	-1.030561	3.774771
154	1	0	2.701158	-1.492775	3.920997
155	1	0	3.084174	-5.775400	3.491136
156	1	0	3.026067	-4.933516	5.044479
157	1	0	1.862240	-4.524205	3.776814
158	6	0	6.952542	-3.110060	3.197812
159	1	0	6.035967	-5.044494	3.290537
160	1	0	5.955486	-4.127497	4.793237
161	6	0	5.043587	3.065613	1.908653
162	6	0	2.537572	2.944510	2.041392
163	1	0	3.899757	1.555121	2.937620
164	6	0	7.822594	-3.381313	2.205283
165	1	0	7.023607	-2.139470	3.693598
166	14	0	5.349683	4.341322	3.317690
167	1	0	5.007121	3.629520	0.966086
168	1	0	5.961218	2.462861	1.861386
169	6	0	1.509930	2.837870	2.895307
170	1	0	2.465537	3.700661	1.256278
171	1	0	7.790328	-4.358913	1.720368
172	6	0	8.855517	-2.464272	1.753661
173	6	0	4.211878	5.847418	3.161579
174	6	0	5.141173	3.517779	5.012291
175	6	0	7.173754	4.902492	3.118711
176	1	0	0.673103	3.522221	2.746843
177	6	0	1.364510	1.913183	4.065218
178	6	0	9.752961	-2.740933	0.793664
179	1	0	8.902519	-1.499281	2.261357
180	1	0	4.480952	6.604766	3.907495
181	1	0	4.293931	6.314122	2.173082
182	1	0	3.162779	5.579357	3.322844
183	1	0	5.778310	2.631349	5.114381
184	1	0	5.419699	4.214904	5.811132
185	1	0	4.103471	3.214164	5.191179
186	6	0	7.475698	5.458693	1.767328
187	1	0	7.828250	4.049803	3.344306
188	1	0	7.358678	5.658535	3.896206
189	1	0	0.460266	1.297402	3.965422
190	1	0	2.216562	1.240589	4.194904
191	1	0	10.526152	-2.031475	0.514337
192	1	0	9.763922	-3.701994	0.283446
193	6	0	8.250619	4.875843	0.832671
194	1	0	7.013491	6.417818	1.524273
195	1	0	8.748691	3.932154	1.066251
196	6	0	8.506843	5.439801	-0.481272
197	6	0	9.299208	4.882972	-1.410656
198	1	0	8.020195	6.391080	-0.701636
199	1	0	9.474231	5.358939	-2.370880
200	1	0	9.823800	3.947258	-1.226048
201	1	0	0.612530	1.845785	-0.727475
202	1	0	0.950201	1.795617	-2.452695
203	1	0	1.244300	2.484872	4.994565
204	1	0	-6.214234	2.688144	2.025174

SIBTS¹

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	-1.461563	0.128346	0.691746
2	7	0	-1.813734	-0.931147	-1.423501
3	6	0	-3.272813	-1.467785	1.071907
4	1	0	-3.223693	-2.522509	0.807782
5	1	0	-3.878702	-1.348896	1.970179
6	6	0	-3.808316	-0.615728	-0.016979

7	6	0	-3.146881	-0.395369	-1.257564
8	6	0	-3.759148	0.384684	-2.253825
9	1	0	-3.267229	0.531230	-3.208849
10	6	0	-5.000166	0.962638	-2.039013
11	1	0	-5.465478	1.545176	-2.828696
12	6	0	-5.647602	0.794812	-0.807720
13	1	0	-6.618734	1.248497	-0.633122
14	6	0	-5.050570	0.035750	0.181254
15	1	0	-5.561598	-0.113671	1.128920
16	6	0	-1.022279	-0.290469	-2.492016
17	1	0	-1.396118	-0.557208	-3.489302
18	1	0	0.010908	-0.632255	-2.410772
19	1	0	-1.039270	0.795230	-2.379251
20	6	0	-1.794298	-2.394020	-1.649048
21	1	0	-2.370057	-2.917897	-0.888167
22	1	0	-0.761200	-2.751302	-1.626397
23	1	0	-2.224330	-2.628732	-2.631423
24	6	0	-0.350968	2.313375	1.099651
25	6	0	-1.210622	2.473480	-0.016276
26	6	0	-2.542599	2.301428	0.428646
27	6	0	-2.507595	2.012319	1.817067
28	6	0	-1.152429	2.039826	2.233430
29	6	0	-1.423615	-1.947196	2.162640
30	6	0	-0.497070	-0.973622	2.574880
31	1	0	-1.110099	-2.681987	1.423749
32	1	0	-2.106015	-2.339994	2.907512
33	6	0	0.650410	-0.589628	1.811608
34	6	0	0.902121	-0.913467	0.495288
35	1	0	1.300662	0.142022	2.290618
36	1	0	0.340269	-1.746155	0.060324
37	1	0	-0.645627	-0.501521	3.541260
38	1	0	-0.900895	2.730290	-1.023004
39	1	0	0.727804	2.408952	1.086278
40	1	0	-0.795905	1.905145	3.246632
41	1	0	-3.368904	1.843941	2.453678
42	1	0	-3.432587	2.378035	-0.182389
43	6	0	2.187479	-0.447010	-0.213142
44	14	0	3.663218	-1.689049	-0.124389
45	1	0	2.551064	0.495560	0.216157
46	1	0	1.999140	-0.252257	-1.279268
47	6	0	4.103951	-2.005125	1.688242
48	6	0	3.188753	-3.309771	-0.987548
49	6	0	5.123647	-0.858022	-1.045980
50	1	0	4.951617	-2.696127	1.764765
51	1	0	4.384874	-1.078589	2.201857
52	1	0	3.265611	-2.452789	2.234247
53	1	0	2.902414	-3.143369	-2.032965
54	1	0	4.033886	-4.007938	-0.987486
55	1	0	2.356047	-3.811383	-0.479556
56	6	0	5.510277	0.448838	-0.435139
57	1	0	4.836657	-0.729541	-2.098248
58	1	0	5.967362	-1.562707	-1.029485
59	6	0	5.221696	1.663628	-0.939580
60	1	0	6.051189	0.399513	0.511872
61	1	0	4.699308	1.732595	-1.896376
62	6	0	5.576738	2.919780	-0.302393
63	6	0	5.292311	4.131564	-0.802546
64	1	0	6.114688	2.848004	0.643901
65	1	0	5.585704	5.043434	-0.291283
66	1	0	4.768680	4.249172	-1.749455

2SIBTS²

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	0.605052	-1.866060	-0.089759
2	6	0	2.353793	-0.233412	1.173206
3	1	0	1.657903	0.598918	1.312873

4	6	0	2.598881	-0.503837	-0.230949
5	6	0	1.778976	-0.145581	-1.277989
6	1	0	2.098538	-0.412162	-2.282631
7	6	0	-0.223795	-4.126373	-0.559657
8	6	0	1.178174	-4.148982	-0.765206
9	6	0	1.474669	-3.305888	-1.862712
10	6	0	0.255055	-2.751329	-2.330102
11	6	0	-0.794951	-3.258832	-1.522946
12	1	0	3.497168	-1.074238	-0.470912
13	6	0	1.358424	-1.553528	2.388941
14	6	0	0.291910	-2.460864	2.073014
15	1	0	1.081339	-0.682722	2.983179
16	1	0	2.252384	-2.046806	2.759883
17	6	0	-1.029661	-2.041214	1.721310
18	6	0	-1.373478	-0.760180	1.343662
19	1	0	-1.778737	-2.821723	1.595189
20	1	0	-0.672595	0.046404	1.580640
21	1	0	0.476651	-3.524058	2.197098
22	6	0	0.524470	0.663788	-1.157693
23	6	0	0.027237	1.229182	-2.498736
24	1	0	-0.333093	0.080206	-0.710599
25	1	0	0.649042	1.495180	-0.450190
26	1	0	0.822637	1.867510	-2.898393
27	1	0	-0.099689	0.408492	-3.214946
28	6	0	-1.280595	1.975172	-2.365462
29	6	0	-1.369303	3.204477	-1.672310
30	6	0	-2.447549	1.408753	-2.886620
31	7	0	-0.171826	3.802786	-1.173178
32	6	0	-2.627257	3.791270	-1.487494
33	6	0	-3.694612	2.008064	-2.712231
34	1	0	-2.377036	0.473548	-3.439506
35	6	0	-0.322722	4.614055	0.026232
36	6	0	0.576414	4.538101	-2.194929
37	1	0	-2.706615	4.735361	-0.957036
38	6	0	-3.782223	3.198066	-1.996255
39	1	0	-4.584637	1.549800	-3.134130
40	1	0	-0.816466	5.585116	-0.151312
41	1	0	0.672195	4.825841	0.433595
42	1	0	-0.896244	4.066707	0.780206
43	1	0	0.673267	3.944302	-3.106783
44	1	0	1.580501	4.765176	-1.819837
45	1	0	0.084177	5.487539	-2.465546
46	1	0	-4.744281	3.682357	-1.850808
47	1	0	-0.764736	-4.688730	0.191089
48	1	0	-1.850159	-3.034073	-1.631631
49	1	0	1.897516	-4.722984	-0.190998
50	1	0	2.462565	-3.119464	-2.268701
51	1	0	0.141490	-2.083960	-3.175994
52	6	0	3.594962	-0.117423	2.040195
53	14	0	4.777213	1.386838	1.717754
54	1	0	4.203478	-1.026649	1.935140
55	6	0	3.921450	2.738685	0.703832
56	6	0	5.295689	2.068681	3.405440
57	6	0	6.349728	0.752275	0.816241
58	1	0	4.600240	3.588088	0.563018
59	1	0	3.617643	2.386657	-0.287857
60	1	0	3.030052	3.116454	1.218720
61	1	0	5.766979	1.295800	4.023649
62	1	0	6.016929	2.886144	3.291750
63	1	0	4.434847	2.461994	3.959027
64	6	0	6.097385	0.141597	-0.519211
65	1	0	6.847117	0.037354	1.485356
66	1	0	7.021597	1.617969	0.722287
67	6	0	6.153135	-1.174255	-0.806912
68	1	0	5.830345	0.830801	-1.323312
69	1	0	6.440487	-1.881129	-0.025716
70	6	0	5.864672	-1.731580	-2.118048
71	6	0	5.874284	-3.042524	-2.412009
72	1	0	5.640107	-1.013448	-2.908899

73	1	0	5.674728	-3.402975	-3.416853
74	1	0	6.119178	-3.793031	-1.662850
75	1	0	3.306870	-0.059796	3.097950
76	6	0	-2.741686	-0.343451	0.924417
77	14	0	-3.847229	0.338162	2.356683
78	1	0	-3.295042	-1.187205	0.492577
79	1	0	-2.702621	0.442885	0.159278
80	6	0	-3.920654	-0.924712	3.762901
81	6	0	-3.147474	1.988994	2.970303
82	6	0	-5.579313	0.602300	1.580897
83	1	0	-4.576279	-0.569075	4.566433
84	1	0	-4.312501	-1.888347	3.418141
85	1	0	-2.930996	-1.099588	4.200084
86	1	0	-3.084350	2.719350	2.155250
87	1	0	-3.789306	2.416331	3.749408
88	1	0	-2.146570	1.870776	3.402865
89	6	0	-6.196344	-0.680075	1.128471
90	1	0	-5.468124	1.303475	0.743208
91	1	0	-6.209727	1.096165	2.333720
92	6	0	-6.250167	-1.116492	-0.144573
93	1	0	-6.609632	-1.319990	1.910348
94	1	0	-5.855545	-0.482070	-0.941169
95	6	0	-6.820724	-2.389616	-0.548735
96	6	0	-6.878489	-2.829162	-1.814829
97	1	0	-7.228011	-3.012717	0.248694
98	1	0	-7.322364	-3.787484	-2.066879
99	1	0	-6.495567	-2.235423	-2.642834

3SIBTS³

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	1.662160	2.122444	-0.977777
2	6	0	-0.821369	2.792153	-0.100419
3	1	0	-0.795237	2.146554	0.781217
4	6	0	-0.743025	2.033645	-1.333567
5	6	0	-0.253044	0.752983	-1.474828
6	1	0	-0.257399	0.318330	-2.470098
7	6	0	3.685083	2.883643	-2.121456
8	6	0	2.591711	3.173348	-2.975856
9	6	0	2.025412	1.942901	-3.390916
10	6	0	2.755779	0.892759	-2.780162
11	6	0	3.781394	1.476258	-1.993948
12	1	0	-1.052601	2.553713	-2.242114
13	6	0	0.710906	4.030659	0.535977
14	6	0	2.127013	3.889573	0.371338
15	1	0	0.324884	3.839828	1.536957
16	1	0	0.300629	4.931152	0.087629
17	6	0	2.902848	2.862870	0.998036
18	6	0	2.379094	1.711505	1.545609
19	1	0	3.984923	2.925579	0.890324
20	1	0	1.304551	1.689797	1.754302
21	1	0	2.650775	4.661621	-0.184208
22	6	0	0.165585	-0.134613	-0.341036
23	6	0	-0.069258	-1.660084	-0.575825
24	1	0	1.255023	-0.023958	-0.087675
25	1	0	-0.353286	0.152169	0.582229
26	1	0	4.342830	3.611225	-1.662782
27	1	0	4.522194	0.936034	-1.415581
28	1	0	2.260841	4.162191	-3.275576
29	1	0	1.184956	1.827646	-4.065501
30	1	0	2.586738	-0.168686	-2.912127
31	6	0	-1.922973	3.827007	-0.036206
32	14	0	-3.719314	3.138450	0.123968
33	1	0	-1.899761	4.477546	-0.921159
34	6	0	-4.221199	2.165569	-1.421265
35	6	0	-3.840582	2.046263	1.667849
36	6	0	-4.830564	4.685254	0.324271

37	1	0	-5.271507	1.859431	-1.346760
38	1	0	-4.117348	2.768843	-2.330314
39	1	0	-3.624113	1.255303	-1.545850
40	1	0	-3.541306	2.590319	2.571450
41	1	0	-4.872116	1.706422	1.815813
42	1	0	-3.215683	1.148834	1.587847
43	6	0	-4.778029	5.584260	-0.868381
44	1	0	-4.514608	5.217494	1.231493
45	1	0	-5.856745	4.333491	0.503197
46	6	0	-4.107123	6.749405	-0.941800
47	1	0	-5.316315	5.243154	-1.754811
48	1	0	-3.579655	7.117493	-0.059113
49	6	0	-4.046856	7.584515	-2.128828
50	6	0	-3.382427	8.747093	-2.205364
51	1	0	-4.590381	7.223946	-3.003261
52	1	0	-3.373436	9.340451	-3.114688
53	1	0	-2.836050	9.148911	-1.354240
54	1	0	-1.781417	4.484574	0.832454
55	6	0	3.187121	0.624982	2.170314
56	14	0	3.469047	0.847885	4.071988
57	1	0	4.185546	0.561112	1.719427
58	1	0	2.705825	-0.352555	2.036134
59	6	0	4.252958	2.537910	4.398152
60	6	0	1.814444	0.684706	4.981407
61	6	0	4.657420	-0.562479	4.592650
62	1	0	4.444437	2.672184	5.469225
63	1	0	5.209983	2.644061	3.874917
64	1	0	3.598874	3.356252	4.076400
65	1	0	1.334611	-0.278512	4.772654
66	1	0	1.960743	0.753360	6.065586
67	1	0	1.116046	1.481047	4.697080
68	6	0	5.990583	-0.453552	3.928285
69	1	0	4.177279	-1.521974	4.358599
70	1	0	4.761243	-0.516226	5.686130
71	6	0	6.415094	-1.204059	2.893829
72	1	0	6.656990	0.322765	4.309007
73	1	0	5.770196	-1.998262	2.511224
74	6	0	7.705167	-1.046770	2.245026
75	6	0	8.132699	-1.791789	1.214816
76	1	0	8.355485	-0.266379	2.642578
77	1	0	9.110470	-1.639989	0.767716
78	1	0	7.521320	-2.588131	0.794523
79	6	0	0.764818	-2.227298	-1.731912
80	14	0	0.413218	-4.034434	-2.284798
81	1	0	1.835433	-2.157233	-1.487785
82	1	0	0.624693	-1.621099	-2.638777
83	6	0	1.037667	-5.306653	-1.029256
84	6	0	-1.440643	-4.257336	-2.609092
85	6	0	1.363015	-4.257873	-3.939132
86	1	0	0.911201	-6.321737	-1.424479
87	1	0	2.102387	-5.167920	-0.808565
88	1	0	0.487512	-5.243788	-0.085104
89	1	0	-1.801456	-3.542649	-3.358723
90	1	0	-1.638917	-5.264512	-2.994677
91	1	0	-2.039577	-4.126246	-1.699833
92	6	0	2.818545	-3.952852	-3.822611
93	1	0	0.891907	-3.621786	-4.700670
94	1	0	1.209906	-5.300161	-4.255960
95	6	0	3.445446	-2.892522	-4.367711
96	1	0	3.413165	-4.648476	-3.226436
97	1	0	2.876084	-2.200926	-4.993031
98	6	0	4.861036	-2.608726	-4.205972
99	6	0	5.497751	-1.563573	-4.756724
100	1	0	5.428130	-3.313960	-3.596383
101	1	0	6.562381	-1.404397	-4.613906
102	1	0	4.975869	-0.844231	-5.384918
103	6	0	0.217972	-2.383251	0.717404
104	6	0	-0.659079	-2.734311	1.668329
105	1	0	1.271569	-2.619476	0.882057

106	1	0	-0.257833	-3.242361	2.547688
107	6	0	-2.144835	-2.530020	1.688164
108	6	0	-2.916894	-3.828834	2.004210
109	1	0	-2.393740	-1.789143	2.463271
110	1	0	-2.512491	-2.123818	0.739238
111	1	0	-2.694808	-4.560766	1.224248
112	1	0	-2.545260	-4.242332	2.951246
113	6	0	-4.401932	-3.573750	2.112927
114	6	0	-5.269399	-3.713638	1.008501
115	6	0	-4.924430	-3.104029	3.321817
116	7	0	-4.749721	-4.226388	-0.222822
117	6	0	-6.615410	-3.351469	1.147502
118	6	0	-6.264973	-2.748706	3.454471
119	1	0	-4.257848	-3.007182	4.177541
120	6	0	-5.384350	-3.720472	-1.429316
121	6	0	-4.690229	-5.687285	-0.244027
122	1	0	-7.290715	-3.461311	0.303917
123	6	0	-7.110706	-2.863680	2.355098
124	1	0	-6.642736	-2.386076	4.406664
125	1	0	-6.394375	-4.129578	-1.611192
126	1	0	-4.764276	-3.988740	-2.292393
127	1	0	-5.457440	-2.629769	-1.381703
128	1	0	-4.193580	-6.061935	0.654920
129	1	0	-4.117700	-6.016842	-1.118606
130	1	0	-5.692839	-6.147466	-0.292855
131	1	0	-8.160178	-2.592513	2.437304
132	1	0	-1.134927	-1.760768	-0.817709

2SIB2SIBTS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	21	0	5.252307	1.807809	0.301568
2	6	0	7.085503	-0.382356	-1.063094
3	1	0	6.283411	-1.064857	-0.751850
4	6	0	7.553793	0.431393	0.109775
5	6	0	7.069228	0.461741	1.375237
6	1	0	7.588991	1.103292	2.086421
7	6	0	3.650574	3.564079	0.760733
8	6	0	4.768882	4.169166	0.129130
9	6	0	5.880695	4.044064	0.999879
10	6	0	5.451021	3.367403	2.168965
11	6	0	4.072305	3.065903	2.019187
12	1	0	8.409094	1.079046	-0.089238
13	6	0	6.564307	0.546825	-2.206006
14	6	0	5.505650	1.636471	-1.972827
15	1	0	6.210521	-0.123863	-3.002881
16	1	0	7.446241	1.057550	-2.609805
17	6	0	4.122479	1.390522	-1.761467
18	6	0	3.591427	0.434407	-0.902632
19	1	0	3.439860	2.185058	-2.071968
20	1	0	4.216678	-0.439123	-0.673269
21	1	0	5.706423	2.533351	-2.556570
22	6	0	5.927396	-0.350131	1.935049
23	1	0	5.034560	0.260352	2.193948
24	1	0	5.611473	-1.171030	1.287002
25	1	0	2.647115	3.501435	0.357333
26	1	0	3.445173	2.569879	2.752516
27	1	0	4.772142	4.654982	-0.838913
28	1	0	6.884814	4.406587	0.807350
29	1	0	6.064120	3.139249	3.033588
30	6	0	8.247372	-1.232266	-1.634621
31	14	0	9.089395	-2.654911	-0.633921
32	1	0	9.044367	-0.549798	-1.964686
33	6	0	7.968822	-3.306173	0.751636
34	6	0	9.453821	-4.041024	-1.867883
35	6	0	10.757068	-2.031151	0.081676
36	1	0	8.419867	-4.196601	1.205025

37	1	0	7.824429	-2.572847	1.552373
38	1	0	6.984626	-3.605015	0.370311
39	1	0	10.068525	-3.684250	-2.702371
40	1	0	9.998421	-4.860169	-1.384649
41	1	0	8.530979	-4.459285	-2.286880
42	6	0	10.625907	-0.938633	1.085177
43	1	0	11.377414	-1.712631	-0.766677
44	1	0	11.253881	-2.905179	0.526247
45	6	0	10.885515	0.366586	0.870392
46	1	0	10.273688	-1.233499	2.076171
47	1	0	11.265271	0.684234	-0.102996
48	6	0	10.701312	1.403994	1.871118
49	6	0	10.876542	2.718998	1.655133
50	1	0	10.414503	1.065853	2.868944
51	1	0	10.752464	3.448756	2.449898
52	1	0	11.199438	3.100071	0.688090
53	1	0	7.870278	-1.700082	-2.555303
54	6	0	2.120048	0.252538	-0.639521
55	14	0	1.326263	-1.060333	-1.813602
56	1	0	1.590240	1.204749	-0.778403
57	1	0	1.940028	-0.065775	0.397108
58	6	0	1.487803	-0.474509	-3.602425
59	6	0	2.193044	-2.724884	-1.561826
60	1	0	1.082768	-1.219811	-4.296982
61	1	0	0.960544	0.470284	-3.776349
62	1	0	2.539426	-0.322253	-3.870421
63	1	0	2.136963	-3.061422	-0.519792
64	1	0	1.733144	-3.501391	-2.183921
65	1	0	3.250600	-2.672934	-1.845878
66	1	0	6.218939	-0.776999	2.901646
67	6	0	-0.538703	-1.329463	-1.378797
68	6	0	-1.445606	-0.147330	-1.553632
69	1	0	-0.854147	-2.155780	-2.031350
70	6	0	-1.927300	0.291031	-2.769477
71	1	0	-1.530756	0.526129	-0.695610
72	6	0	-2.841678	1.375222	-2.945151
73	1	0	-1.732429	-0.328385	-3.644292
74	21	0	-4.119177	-0.064034	-1.726687
75	6	0	-3.137934	2.349376	-1.935959
76	1	0	-3.277080	1.520555	-3.928972
77	6	0	-5.216102	1.188199	0.050362
78	6	0	-5.822058	-0.302241	-3.452555
79	1	0	-2.298477	2.684447	-1.327170
80	1	0	-3.757975	3.168819	-2.287391
81	6	0	-4.143100	2.146941	-0.128123
82	6	0	-5.085624	-0.113975	0.479717
83	1	0	-6.215795	1.523460	-0.231642
84	6	0	-4.653470	-0.935490	-3.945505
85	6	0	-6.277788	-1.040625	-2.332475
86	1	0	-6.299136	0.575507	-3.875774
87	1	0	-3.250790	1.881100	0.444789
88	6	0	-4.533625	3.599359	0.018176
89	1	0	-5.988794	-0.710443	0.568205
90	6	0	-3.807132	-0.735187	0.955342
91	6	0	-4.376716	-2.050164	-3.116034
92	1	0	-4.089578	-0.634382	-4.819463
93	6	0	-5.382436	-2.117888	-2.118894
94	1	0	-7.167125	-0.824982	-1.751893
95	14	0	-4.956511	4.206989	1.804556
96	1	0	-5.406253	3.831529	-0.607808
97	1	0	-3.721660	4.253510	-0.328050
98	6	0	-3.982207	-1.843487	2.040813
99	1	0	-3.218672	-1.207164	0.119757
100	1	0	-3.132132	0.034394	1.351513
101	1	0	-3.560525	-2.752631	-3.240828
102	1	0	-5.470999	-2.884864	-1.359489
103	6	0	-6.386258	3.217816	2.552886
104	6	0	-3.407957	4.058063	2.890255
105	6	0	-5.454348	6.041180	1.592445

106	6	0	-4.748747	-3.071251	1.530723
107	6	0	-2.615561	-2.222073	2.554128
108	1	0	-4.556609	-1.376202	2.850357
109	1	0	-6.666837	3.645179	3.523067
110	1	0	-7.276629	3.245711	1.914662
111	1	0	-6.121852	2.168431	2.724060
112	1	0	-2.565268	4.617827	2.467520
113	1	0	-3.603021	4.464820	3.889309
114	1	0	-3.094335	3.015068	3.021462
115	6	0	-6.682973	6.198475	0.754542
116	1	0	-4.606654	6.583449	1.152523
117	1	0	-5.610946	6.459134	2.597180
118	14	0	-5.181462	-4.454664	2.800816
119	1	0	-4.188226	-3.544468	0.710481
120	1	0	-5.712646	-2.766889	1.098117
121	6	0	-2.028338	-1.827598	3.692422
122	1	0	-2.061877	-2.905924	1.906666
123	6	0	-6.707508	6.612228	-0.526635
124	1	0	-7.629430	5.935872	1.230553
125	6	0	-3.676850	-5.535698	3.192501
126	6	0	-5.889694	-3.690097	4.382459
127	6	0	-6.530545	-5.523138	1.954060
128	1	0	-1.031046	-2.221066	3.894901
129	6	0	-2.572796	-0.924031	4.755771
130	1	0	-5.772496	6.903285	-1.010751
131	6	0	-7.914587	6.729131	-1.326665
132	1	0	-3.971748	-6.375764	3.832505
133	1	0	-3.230952	-5.954832	2.282961
134	1	0	-2.901927	-4.971310	3.721127
135	1	0	-6.746693	-3.039206	4.172790
136	1	0	-6.236167	-4.477135	5.062298
137	1	0	-5.138382	-3.102046	4.921820
138	6	0	-6.114624	-6.039152	0.617149
139	1	0	-7.450804	-4.929053	1.873969
140	1	0	-6.750167	-6.356739	2.637480
141	1	0	-1.916679	-0.055653	4.901226
142	1	0	-3.578081	-0.552618	4.538693
143	6	0	-7.939549	7.148336	-2.600363
144	1	0	-8.850777	6.460065	-0.835988
145	6	0	-6.629439	-5.658679	-0.568136
146	1	0	-5.315786	-6.783979	0.612956
147	1	0	-8.868760	7.230103	-3.155957
148	1	0	-7.030713	7.440500	-3.123064
149	1	0	-7.455153	-4.943537	-0.585696
150	6	0	-6.184456	-6.171084	-1.853133
151	6	0	-6.705846	-5.816954	-3.038052
152	1	0	-5.377671	-6.905289	-1.826880
153	1	0	-6.348922	-6.246129	-3.969456
154	1	0	-7.527033	-5.106485	-3.110983
155	1	0	-2.608691	-1.445334	5.720865
156	1	0	-0.593177	-1.711249	-0.351543
