Supporting Information

Theoretical investigation on the mechanism of gold(I)-catalyzed hydrothiolation of alkynes and alkenes with phenthiol

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The Cartesian coordinates of the stationary points discussed in the text

RC1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.677085	-3.029678	0.265311
2	6	0	-0.676562	-3.029723	0.265360
3	7	0	-1.079680	-1.700593	0.175320
4	6	0	0.000181	-0.864650	0.107733
5	7	0	1.080062	-1.700479	0.175269
6	79	0	-0.000146	1.137177	-0.098624
7	1	0	1.386931	-3.835532	0.354091
8	1	0	-1.386297	-3.835687	0.354045
9	6	0	-2.457203	-1.298853	0.127372
10	6	0	-2.932386	-0.311490	0.993247
11	6	0	-3.312098	-1.928345	-0.780416
12	6	0	-4.277129	0.054399	0.934908
13	1	0	-2.256622	0.164615	1.694213
14	6	0	-4.657781	-1.563111	-0.820667
15	1	0	-2.921517	-2.678500	-1.461042
16	6	0	-5.141117	-0.570202	0.033405
17	1	0	-4.647253	0.828043	1.600107
18	1	0	-5.322869	-2.046383	-1.529657
19	1	0	-6.186996	-0.281774	-0.005683
20	6	0	2.457523	-1.298579	0.127350
21	6	0	2.932399	-0.310592	0.992669
22	6	0	3.312700	-1.928494	-0.779891
23	6	0	4.277105	0.055463	0.934359
24	1	0	2.256446	0.165892	1.693199
25	6	0	4.658328	-1.563093	-0.820111

26	1	0	2.922378	-2.679139	-1.460129
27	6	0	5.141368	-0.569574	0.033431
28	1	0	4.646948	0.829594	1.599148
29	1	0	5.323610	-2.046725	-1.528675
30	1	0	6.187214	-0.281029	-0.005633
31	17	0	-0.000447	3.447429	-0.332423

1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.230156	0.659720	-2.067603
2	6	0	2.612961	1.864974	-2.081990
3	7	0	1.623158	1.823375	-1.105226
4	6	0	1.615675	0.614342	-0.470358
5	7	0	2.606607	-0.099643	-1.082301
6	79	0	0.426818	0.032952	1.045642
7	1	0	4.022034	0.259397	-2.679035
8	1	0	2.757570	2.729274	-2.709033
9	6	0	0.759522	2.933336	-0.809516
10	6	0	-0.624494	2.754397	-0.763713
11	6	0	1.329918	4.189833	-0.591020
12	6	0	-1.441443	3.849064	-0.480006
13	6	0	0.501557	5.279511	-0.322386
14	6	0	-0.883288	5.110209	-0.263027
15	1	0	-2.515742	3.703294	-0.432184
16	1	0	0.941792	6.256200	-0.146431
17	1	0	-1.524919	5.958523	-0.045194
18	6	0	2.992864	-1.444332	-0.759757
19	6	0	2.037360	-2.462646	-0.742438
20	6	0	4.336311	-1.715047	-0.490430
21	6	0	2.436805	-3.763626	-0.436093
22	6	0	4.725677	-3.022162	-0.197532
23	6	0	3.777302	-4.046238	-0.166284
24	1	0	1.696112	-4.556676	-0.414478
25	1	0	5.768095	-3.235081	0.018211
26	1	0	4.081754	-5.061316	0.069309
27	16	0	-3.869706	0.628183	0.458551
28	1	0	-2.965012	0.223174	1.381341
29	17	0	-1.001656	-0.630313	2.773384
30	6	0	-3.975775	-0.909503	-0.447838
31	6	0	-3.376121	-2.092243	0.009208
32	6	0	-4.703929	-0.922014	-1.646037

33	6	0	-3.505646	-3.266721	-0.733970
34	1	0	-2.812934	-2.093084	0.937441
35	6	0	-4.830688	-2.103194	-2.376507
36	1	0	-5.171270	-0.009199	-2.005262
37	6	0	-4.231391	-3.281450	-1.926652
38	1	0	-3.039604	-4.177891	-0.368118
39	1	0	-5.400114	-2.099596	-3.302073
40	1	0	-4.332022	-4.200074	-2.497161
41	1	0	5.061767	-0.907390	-0.490285
42	1	0	1.000587	-2.235423	-0.963025
43	1	0	-1.060856	1.777448	-0.937722
44	1	0	2.409224	4.306244	-0.610026

TSa1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.098029	3.166634	0.213650
2	6	0	3.185776	2.362684	0.169973
3	7	0	2.716166	1.052953	0.116323
4	6	0	1.349111	1.019900	0.115097
5	7	0	0.981019	2.335459	0.185874
6	79	0	0.135439	-0.618218	-0.006142
7	1	0	2.010580	4.237344	0.297470
8	1	0	4.238441	2.590184	0.207066
9	6	0	3.580425	-0.089896	0.039441
10	6	0	3.406537	-1.163544	0.915795
11	6	0	4.606891	-0.098540	-0.908211
12	6	0	4.264046	-2.260234	0.827300
13	6	0	5.466498	-1.194924	-0.978458
14	6	0	5.294622	-2.277997	-0.114598
15	1	0	4.125763	-3.099323	1.501828
16	1	0	6.260816	-1.205911	-1.718431
17	1	0	5.959698	-3.133798	-0.176826
18	6	0	-0.366093	2.829574	0.194693
19	6	0	-1.310011	2.289068	1.071004
20	6	0	-0.708349	3.871972	-0.670873
21	6	0	-2.611429	2.791636	1.065267
22	6	0	-2.008265	4.377645	-0.655703
23	6	0	-2.961969	3.836918	0.208712
24	1	0	-3.349343	2.362279	1.735121
25	1	0	-2.276304	5.184717	-1.330628
26	1	0	-3.975504	4.225940	0.212099

27	16	0	-1.177131	-2.549411	-0.103521
28	6	0	-2.880199	-2.004808	-0.176965
29	6	0	-3.297349	-0.832602	-0.832268
30	6	0	-3.862143	-2.825463	0.405769
31	6	0	-4.648566	-0.489128	-0.887277
32	1	0	-2.555916	-0.196950	-1.306042
33	6	0	-5.212486	-2.483123	0.337963
34	1	0	-3.556840	-3.733905	0.916510
35	6	0	-5.616074	-1.310663	-0.304699
36	1	0	-4.945027	0.424000	-1.397941
37	1	0	-5.952030	-3.135178	0.796137
38	1	0	-6.667960	-1.043674	-0.354090
39	1	0	0.029798	4.266785	-1.362095
40	1	0	4.715234	0.734386	-1.595979
41	1	0	-1.029897	1.482833	1.739181
42	1	0	2.608570	-1.139455	1.649110

TSa2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.882741	1.850431	0.213608
2	6	0	4.330726	0.640095	0.622091
3	7	0	3.324845	-0.279229	0.333627
4	6	0	2.257591	0.332156	-0.262383
5	7	0	2.611329	1.649831	-0.317241
6	79	0	0.500168	-0.533044	-0.886406
7	1	0	4.324113	2.831227	0.281320
8	1	0	5.241982	0.351556	1.119591
9	6	0	3.418787	-1.676791	0.641621
10	6	0	2.378792	-2.314426	1.324145
11	6	0	4.572101	-2.374500	0.273558
12	6	0	2.501964	-3.671554	1.625802
13	6	0	4.686728	-3.727494	0.593115
14	6	0	3.651374	-4.378487	1.266785
15	1	0	1.694522	-4.170297	2.152871
16	1	0	5.580491	-4.272502	0.304677
17	1	0	3.740543	-5.432895	1.510631
18	6	0	1.787191	2.711743	-0.820949
19	6	0	0.501263	2.895418	-0.307450
20	6	0	2.303634	3.568693	-1.795741
21	6	0	-0.275526	3.949968	-0.788668
22	6	0	1.519756	4.624155	-2.262648

23	6	0	0.230020	4.814674	-1.761616
24	1	0	-1.271470	4.092605	-0.381851
25	1	0	1.915652	5.290566	-3.023101
26	1	0	-0.377578	5.637052	-2.127572
27	16	0	-1.393820	-0.664929	1.312400
28	6	0	-1.773766	0.862630	2.119056
29	6	0	-2.710826	1.766670	1.569897
30	6	0	-1.148979	1.234933	3.329594
31	6	0	-3.007504	2.974758	2.201186
32	1	0	-3.213384	1.499355	0.644785
33	6	0	-1.436694	2.451169	3.948383
34	1	0	-0.438295	0.549474	3.782428
35	6	0	-2.369094	3.331515	3.392619
36	1	0	-3.744861	3.642104	1.759564
37	1	0	-0.935312	2.708483	4.878736
38	1	0	-2.597533	4.274730	3.880735
39	1	0	3.299800	3.398394	-2.192855
40	1	0	5.360505	-1.866675	-0.273641
41	1	0	0.114234	2.233361	0.459375
42	1	0	1.488423	-1.762125	1.609927
43	6	0	-1.131321	-1.460146	-1.864169
44	1	0	-0.855644	-1.832187	-2.850434
45	6	0	-2.297881	-1.527519	-1.378047
46	6	0	-3.667181	-1.662775	-1.066347
47	6	0	-4.582850	-0.649113	-1.436413
48	6	0	-4.155864	-2.848491	-0.467634
49	6	0	-5.942229	-0.817156	-1.201256
50	1	0	-4.205565	0.257105	-1.898483
51	6	0	-5.516565	-3.006253	-0.245309
52	1	0	-3.450077	-3.618036	-0.174663
53	6	0	-6.412378	-1.992256	-0.606481
54	1	0	-6.639332	-0.033250	-1.481721
55	1	0	-5.885322	-3.916784	0.217188
56	1	0	-7.475300	-2.118400	-0.422639

TSa3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.174001	-0.040113	-0.158872
2	6	0	0.084352	-0.097072	1.191195
3	7	0	1.385564	-0.165885	1.679250
4	6	0	2.291237	-0.143632	0.656586

5	7	0	1.528468	-0.076202	-0.473889
6	79	0	4.323204	-0.149162	0.781758
7	1	0	-0.586841	-0.013871	-0.921515
8	1	0	-0.771398	-0.132729	1.845047
9	6	0	1.699289	-0.237280	3.079218
10	6	0	2.569151	-1.222184	3.552736
11	6	0	1.097359	0.675219	3.949802
12	6	0	2.841056	-1.277090	4.920820
13	6	0	1.369411	0.599596	5.315758
14	6	0	2.243161	-0.374723	5.802738
15	1	0	3.519600	-2.038600	5.292558
16	1	0	0.906419	1.309298	5.994666
17	1	0	2.457525	-0.429106	6.865867
18	6	0	2.026962	-0.021908	-1.819660
19	6	0	2.891221	-1.013589	-2.287362
20	6	0	1.608627	1.021513	-2.649790
21	6	0	3.348279	-0.944950	-3.604548
22	6	0	2.065032	1.072752	-3.966645
23	6	0	2.937209	0.091808	-4.444144
24	1	0	4.018338	-1.718363	-3.964851
25	1	0	1.746023	1.884233	-4.613731
26	1	0	3.293880	0.135635	-5.468873
27	16	0	5.200240	-3.050533	1.478516
28	6	0	4.901045	-3.668229	-0.155906
29	6	0	3.715090	-4.376031	-0.448011
30	6	0	5.831828	-3.498321	-1.202027
31	6	0	3.479262	-4.897210	-1.720339
32	1	0	2.986488	-4.523855	0.344025
33	6	0	5.587464	-4.012046	-2.476024
34	1	0	6.755285	-2.962801	-1.004611
35	6	0	4.411225	-4.717538	-2.746939
36	1	0	2.560888	-5.447772	-1.910479
37	1	0	6.328963	-3.870120	-3.259092
38	1	0	4.227970	-5.126970	-3.736340
39	1	0	0.948601	1.791056	-2.260809
40	1	0	0.439228	1.445217	3.558619
41	1	0	3.193518	-1.830755	-1.641895
42	1	0	3.035472	-1.926821	2.868654
43	6	0	6.767782	-0.860306	1.200864
44	1	0	7.363067	-1.657138	1.585026
45	6	0	6.425572	0.292388	0.805599
46	6	0	7.046653	1.583750	0.493173
47	6	0	6.271833	2.722455	0.222139
48	6	0	8.450297	1.697835	0.459939

49	6	0	6.881329	3.943594	-0.064519
50	1	0	5.190473	2.630977	0.241448
51	6	0	9.055213	2.916496	0.166679
52	1	0	9.059456	0.821971	0.662503
53	6	0	8.272820	4.045284	-0.094920
54	1	0	6.266820	4.815882	-0.268586
55	1	0	10.139070	2.987216	0.143158
56	1	0	8.746721	4.995739	-0.323058

3a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.934289	2.539933	0.200680
2	6	0	4.700437	1.436239	0.364961
3	7	0	3.851305	0.339229	0.247307
4	6	0	2.564257	0.731756	0.002306
5	7	0	2.632213	2.097656	-0.015495
6	79	0	0.884426	-0.455736	-0.286663
7	1	0	4.181210	3.587523	0.252079
8	1	0	5.748835	1.327143	0.588989
9	6	0	4.304085	-1.017502	0.352541
10	6	0	3.640838	-1.917784	1.189668
11	6	0	5.430617	-1.413151	-0.373006
12	6	0	4.107875	-3.228677	1.286171
13	6	0	5.896184	-2.723214	-0.258669
14	6	0	5.234646	-3.633376	0.567637
15	1	0	3.589961	-3.931442	1.931347
16	1	0	6.768541	-3.032961	-0.825976
17	1	0	5.594830	-4.654263	0.650163
18	6	0	1.533981	2.989625	-0.264593
19	6	0	0.318607	2.820624	0.402903
20	6	0	1.711358	4.036558	-1.173395
21	6	0	-0.731143	3.702632	0.142082
22	6	0	0.661025	4.922667	-1.412777
23	6	0	-0.561199	4.755318	-0.759103
24	1	0	-1.681243	3.559106	0.646312
25	1	0	0.796607	5.733974	-2.121626
26	1	0	-1.380879	5.439853	-0.954954
27	16	0	-2.121751	-0.351179	1.460678
28	6	0	-3.354177	0.853556	0.980978
29	6	0	-3.710151	1.099414	-0.352525
30	6	0	-3.935560	1.626750	1.999299

31	6	0	-4.637867	2.097205	-0.655371
32	1	0	-3.261260	0.512955	-1.146416
33	6	0	-4.848404	2.633367	1.685414
34	1	0	-3.675757	1.433079	3.036694
35	6	0	-5.208117	2.872197	0.356413
36	1	0	-4.910252	2.271586	-1.692988
37	1	0	-5.289796	3.222945	2.484674
38	1	0	-5.927793	3.648734	0.114126
39	1	0	2.652928	4.141758	-1.703603
40	1	0	5.922738	-0.707556	-1.035279
41	1	0	0.187963	2.002998	1.102445
42	1	0	2.770852	-1.593709	1.748968
43	6	0	-0.792974	-1.582261	-0.577230
44	1	0	-0.760697	-2.391073	-1.313651
45	6	0	-1.990628	-1.468363	0.045260
46	6	0	-3.186507	-2.295066	-0.288626
47	6	0	-3.428666	-2.669472	-1.624016
48	6	0	-4.091876	-2.738976	0.690969
49	6	0	-4.514117	-3.475897	-1.961566
50	1	0	-2.763056	-2.308359	-2.402410
51	6	0	-5.177720	-3.545594	0.353203
52	1	0	-3.932618	-2.451325	1.724943
53	6	0	-5.395009	-3.920993	-0.973780
54	1	0	-4.679302	-3.746068	-3.001298
55	1	0	-5.857144	-3.882216	1.131845
56	1	0	-6.245426	-4.543964	-1.236516

4a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.971100	-3.946801	0.235745
2	6	0	3.122753	-3.348470	-0.149134
3	7	0	2.839419	-1.993470	-0.296519
4	6	0	1.531531	-1.725446	-0.001558
5	7	0	1.006198	-2.946925	0.318054
6	79	0	0.558857	0.108807	-0.012281
7	1	0	1.738938	-4.982388	0.422004
8	1	0	4.096352	-3.756439	-0.365702
9	6	0	3.821776	-1.023993	-0.687599
10	6	0	3.548292	-0.123265	-1.719437
11	6	0	5.058524	-1.013132	-0.037835
12	6	0	4.522351	0.803791	-2.090212

13	6	0	6.029752	-0.090164	-0.426147
14	6	0	5.762790	0.821095	-1.449423
15	1	0	4.308841	1.509795	-2.886587
16	1	0	6.989185	-0.076727	0.081841
17	1	0	6.517508	1.543561	-1.744566
18	6	0	-0.348005	-3.195708	0.727085
19	6	0	-1.414524	-2.652228	0.007535
20	6	0	-0.576222	-4.001842	1.845741
21	6	0	-2.720396	-2.910717	0.426068
22	6	0	-1.886334	-4.267445	2.244252
23	6	0	-2.959310	-3.720172	1.538237
24	1	0	-3.547709	-2.472645	-0.122895
25	1	0	-2.064574	-4.890187	3.115697
26	1	0	-3.978008	-3.919676	1.856469
27	16	0	-2.328053	0.882298	-1.773731
28	6	0	-3.995009	0.680107	-1.157494
29	6	0	-4.950953	0.124203	-2.023669
30	6	0	-4.368663	1.014267	0.152114
31	6	0	-6.254517	-0.097861	-1.582386
32	1	0	-4.672504	-0.123735	-3.044518
33	6	0	-5.681029	0.803607	0.578984
34	1	0	-3.631768	1.433023	0.829763
35	6	0	-6.628830	0.244897	-0.280207
36	1	0	-6.983647	-0.528180	-2.263848
37	1	0	-5.959108	1.072739	1.594666
38	1	0	-7.647665	0.080761	0.058362
39	1	0	0.262595	-4.397037	2.410484
40	1	0	5.248090	-1.705395	0.776706
41	1	0	-1.229835	-2.022657	-0.855186
42	1	0	2.585015	-0.148169	-2.215696
43	6	0	-1.620758	2.087797	-0.671731
44	1	0	-2.181247	3.023297	-0.627565
45	6	0	-0.448236	1.912055	-0.020625
46	6	0	0.112146	3.083747	0.705083
47	6	0	0.726459	2.919977	1.962142
48	6	0	0.055330	4.387075	0.173147
49	6	0	1.227818	4.010340	2.670586
50	1	0	0.796153	1.919258	2.379894
51	6	0	0.568470	5.477752	0.875649
52	1	0	-0.375306	4.536111	-0.812595
53	6	0	1.152235	5.296958	2.130769
54	1	0	1.685565	3.855070	3.644254
55	1	0	0.517863	6.471248	0.437190
56	1	0	1.553853	6.146063	2.676920

P1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.682651	1.875524	-0.698853
2	6	0	1.664555	0.477378	-0.149424
3	6	0	1.611949	-0.000734	1.165594
4	6	0	2.558300	-0.096930	-1.061728
5	6	0	2.435640	-1.056386	1.554495
6	1	0	0.930069	0.451700	1.878056
7	6	0	3.396162	-1.136727	-0.657625
8	1	0	2.592360	0.266300	-2.084525
9	6	0	3.333306	-1.624412	0.648252
10	1	0	2.382643	-1.428047	2.573841
11	1	0	4.088356	-1.574766	-1.370967
12	1	0	3.978050	-2.441381	0.957829
13	6	0	-1.413982	2.697207	0.772771
14	1	0	-2.434793	2.678128	1.142255
15	6	0	-0.896965	1.639689	0.125095
16	6	0	-1.623773	0.352719	-0.032021
17	6	0	-2.422202	-0.130650	1.018820
18	6	0	-1.555583	-0.395554	-1.218050
19	6	0	-3.149752	-1.310781	0.878257
20	1	0	-2.455111	0.416815	1.955837
21	6	0	-2.284129	-1.574918	-1.357440
22	1	0	-0.935336	-0.040046	-2.033924
23	6	0	-3.085574	-2.036965	-0.311966
24	1	0	-3.757851	-1.669236	1.703851
25	1	0	-2.225016	-2.134926	-2.286187
26	1	0	-3.647456	-2.960011	-0.420176
27	1	0	-0.846050	3.609464	0.915579

P2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	1.294830	-1.625844	0.164100
2	6	0	2.585585	-0.393866	0.002515
3	6	0	2.390869	0.807661	-0.690950
4	6	0	3.839377	-0.678938	0.559790
5	6	0	3.439455	1.720631	-0.806671

6	1	0	1.427521	1.022078	-1.142284
7	6	0	4.887448	0.229548	0.418727
8	1	0	3.987836	-1.603921	1.108887
9	6	0	4.690549	1.434829	-0.258020
10	1	0	3.278801	2.652758	-1.340861
11	1	0	5.856318	-0.000043	0.852715
12	1	0	5.505721	2.145082	-0.357144
13	6	0	-1.333094	-0.992058	-0.239948
14	6	0	-0.157097	-0.628466	0.301931
15	1	0	-1.351673	-1.867760	-0.886717
16	6	0	-2.621695	-0.313062	-0.061167
17	6	0	-3.693723	-0.664665	-0.901610
18	6	0	-2.842673	0.682613	0.909655
19	6	0	-4.931466	-0.034382	-0.793733
20	1	0	-3.545537	-1.437680	-1.651299
21	6	0	-4.077743	1.314885	1.014447
22	1	0	-2.047957	0.951290	1.598795
23	6	0	-5.128588	0.961937	0.163067
24	1	0	-5.742315	-0.322374	-1.456566
25	1	0	-4.226125	2.079569	1.771576
26	1	0	-6.092949	1.453042	0.252236
27	1	0	-0.050139	0.261467	0.916855

TSb2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.405203	1.557142	2.135784
2	6	0	3.999636	0.362452	1.902352
3	7	0	3.301582	-0.235712	0.857651
4	6	0	2.289395	0.568201	0.423888
5	7	0	2.355232	1.666812	1.229281
6	79	0	0.933375	0.192535	-1.062951
7	1	0	3.601543	2.316403	2.874891
8	1	0	4.819975	-0.131963	2.396196
9	6	0	3.597661	-1.547096	0.352070
10	6	0	2.591863	-2.516463	0.307365
11	6	0	4.901610	-1.836450	-0.056158
12	6	0	2.908049	-3.789682	-0.169435
13	6	0	5.204419	-3.116851	-0.519841
14	6	0	4.207859	-4.093245	-0.579780
15	1	0	2.131343	-4.547207	-0.207330
16	1	0	6.215653	-3.345701	-0.842174

17	1	0	4.444810	-5.088412	-0.944066
18	6	0	1.445451	2.777923	1.196279
19	6	0	0.069974	2.550502	1.294166
20	6	0	1.961050	4.071986	1.094489
21	6	0	-0.794762	3.646267	1.271143
22	6	0	1.085000	5.157697	1.087046
23	6	0	-0.292816	4.945663	1.171201
24	1	0	-1.864555	3.474568	1.336211
25	1	0	1.480217	6.165674	1.004998
26	1	0	-0.972960	5.792267	1.160467
27	16	0	-1.178625	-1.249494	0.924071
28	6	0	-2.708810	-2.015049	1.339328
29	6	0	-3.715520	-1.313783	2.041064
30	6	0	-2.993540	-3.345431	0.953966
31	6	0	-4.935089	-1.915545	2.349103
32	1	0	-3.518588	-0.291128	2.347334
33	6	0	-4.216951	-3.940653	1.256511
34	1	0	-2.230935	-3.906543	0.421153
35	6	0	-5.197377	-3.231120	1.957601
36	1	0	-5.686986	-1.352362	2.897181
37	1	0	-4.405453	-4.966446	0.948179
38	1	0	-6.148781	-3.697859	2.197030
39	1	0	3.032735	4.222468	1.005184
40	1	0	5.662820	-1.062657	-0.025875
41	1	0	-0.317726	1.538863	1.388005
42	1	0	1.583848	-2.282767	0.640442
43	6	0	-2.814373	0.351900	-1.542222
44	6	0	-2.691073	1.749951	-1.701490
45	6	0	-4.070535	-0.172680	-1.170889
46	6	0	-3.784369	2.584070	-1.501893
47	1	0	-1.728433	2.178030	-1.961674
48	6	0	-5.165195	0.666906	-0.981152
49	1	0	-4.177467	-1.243097	-1.031776
50	6	0	-5.027619	2.046481	-1.145867
51	1	0	-3.672486	3.657714	-1.625684
52	1	0	-6.123188	0.242555	-0.696481
53	1	0	-5.880983	2.701804	-0.995765
54	6	0	-0.550928	-0.237960	-2.572328
55	1	0	-0.605231	0.671619	-3.170732
56	1	0	-0.117501	-1.081068	-3.112978
57	6	0	-1.720014	-0.563642	-1.823679
58	1	0	-1.927188	-1.609783	-1.634954

TSb3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.676874	0.339542	-2.163698
2	6	0	-3.980417	-0.851400	-1.594007
3	7	0	-3.010732	-1.091861	-0.625466
4	6	0	-2.114702	-0.065547	-0.569912
5	7	0	-2.527376	0.805984	-1.533299
6	79	0	-0.510427	0.109402	0.671063
7	1	0	-4.140722	0.879173	-2.972916
8	1	0	-4.762813	-1.561606	-1.805587
9	6	0	-2.958941	-2.286588	0.170094
10	6	0	-1.791250	-3.054202	0.194695
11	6	0	-4.095022	-2.672984	0.884513
12	6	0	-1.770112	-4.219289	0.963055
13	6	0	-4.061887	-3.845884	1.639135
14	6	0	-2.899130	-4.617839	1.681912
15	1	0	-0.866364	-4.820316	0.987804
16	1	0	-4.941030	-4.148274	2.199865
17	1	0	-2.873934	-5.528448	2.272894
18	6	0	-1.864284	2.027952	-1.895609
19	6	0	-0.507364	2.010117	-2.228251
20	6	0	-2.605726	3.210671	-1.940763
21	6	0	0.108969	3.206111	-2.599033
22	6	0	-1.978208	4.395917	-2.324146
23	6	0	-0.620669	4.395263	-2.650957
24	1	0	1.163481	3.199498	-2.856192
25	1	0	-2.548801	5.319009	-2.356147
26	1	0	-0.133199	5.319922	-2.944798
27	16	0	1.630683	-1.303259	-1.217474
28	6	0	3.278753	-1.942034	-1.300751
29	6	0	3.554813	-3.291076	-0.994784
30	6	0	4.367773	-1.110119	-1.635069
31	6	0	4.857813	-3.785316	-1.030236
32	1	0	2.728217	-3.947402	-0.738491
33	6	0	5.670928	-1.606940	-1.666582
34	1	0	4.174153	-0.070455	-1.883373
35	6	0	5.924858	-2.946912	-1.364946
36	1	0	5.042049	-4.830742	-0.794480
37	1	0	6.491621	-0.944357	-1.930725
38	1	0	6.939867	-3.333266	-1.391187
39	1	0	-3.655007	3.203228	-1.661672
40	1	0	-4.985571	-2.052183	0.862292

41	1	0	0.057105	1.082408	-2.199087
42	1	0	-0.917289	-2.747876	-0.374099
43	6	0	1.510193	1.791115	2.169306
44	6	0	2.234037	2.520003	1.207347
45	6	0	1.067969	2.474097	3.316626
46	6	0	2.511005	3.873295	1.395484
47	1	0	2.570347	2.026547	0.300060
48	6	0	1.343360	3.827497	3.501912
49	1	0	0.505493	1.930111	4.072039
50	6	0	2.068622	4.537092	2.542044
51	1	0	3.074282	4.413409	0.638879
52	1	0	0.993362	4.328205	4.400786
53	1	0	2.285228	5.591778	2.684922
54	6	0	1.220933	0.337024	2.022960
55	1	0	0.773225	-0.126337	2.905592
56	6	0	2.047401	-0.522890	1.259334
57	1	0	2.040793	-1.584559	1.467245
58	1	0	2.928031	-0.147020	0.755307

3b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.037507	2.592186	0.175231
2	6	0	4.806964	1.505682	0.417949
3	7	0	3.971653	0.395237	0.323019
4	6	0	2.689768	0.760682	0.015479
5	7	0	2.747590	2.125500	-0.064473
6	79	0	1.027222	-0.459988	-0.299312
7	1	0	4.273168	3.643623	0.186301
8	1	0	5.847850	1.418560	0.683033
9	6	0	4.432941	-0.950006	0.505579
10	6	0	3.745990	-1.820370	1.355160
11	6	0	5.590689	-1.364828	-0.157429
12	6	0	4.221809	-3.120183	1.528131
13	6	0	6.064041	-2.663257	0.032683
14	6	0	5.379685	-3.543570	0.872555
15	1	0	3.686271	-3.799734	2.183792
16	1	0	6.960776	-2.987718	-0.486351
17	1	0	5.746261	-4.555621	1.014529
18	6	0	1.648869	2.991275	-0.387359
19	6	0	0.414617	2.833394	0.247424
20	6	0	1.841772	4.002172	-1.333151

21	6	0	-0.636439	3.689320	-0.083929
22	6	0	0.788811	4.863077	-1.643222
23	6	0	-0.452079	4.706292	-1.022746
24	1	0	-1.599675	3.552448	0.397519
25	1	0	0.937416	5.646274	-2.380491
26	1	0	-1.272509	5.372446	-1.272132
27	16	0	-2.111458	-0.189380	1.181336
28	6	0	-3.689167	0.649639	1.244413
29	6	0	-4.271142	1.290158	0.139738
30	6	0	-4.332848	0.728998	2.489761
31	6	0	-5.473814	1.983757	0.280812
32	1	0	-3.790066	1.247688	-0.831321
33	6	0	-5.523402	1.441700	2.628247
34	1	0	-3.899013	0.222415	3.347176
35	6	0	-6.103678	2.068723	1.523754
36	1	0	-5.916355	2.465069	-0.587419
37	1	0	-6.006452	1.492541	3.600403
38	1	0	-7.037620	2.612980	1.629256
39	1	0	2.798718	4.098540	-1.836861
40	1	0	6.101529	-0.683601	-0.830936
41	1	0	0.269138	2.043870	0.975303
42	1	0	2.851076	-1.481683	1.864217
43	6	0	-3.195006	-1.864372	-0.821456
44	6	0	-3.916443	-1.702450	-2.011302
45	6	0	-3.547269	-2.922300	0.030578
46	6	0	-4.956716	-2.571917	-2.348453
47	1	0	-3.656764	-0.888799	-2.685057
48	6	0	-4.585790	-3.789807	-0.300741
49	1	0	-3.007468	-3.052844	0.963868
50	6	0	-5.295871	-3.619318	-1.493095
51	1	0	-5.502770	-2.426059	-3.276739
52	1	0	-4.845163	-4.601274	0.374182
53	1	0	-6.107077	-4.295393	-1.748651
54	6	0	-0.653678	-1.659553	-0.621582
55	1	0	-0.598910	-2.087581	-1.631683
56	1	0	-0.647129	-2.515785	0.065751
57	6	0	-2.022138	-0.948076	-0.521143
58	1	0	-2.035026	-0.118699	-1.234500

4b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.841354	3.934826	0.323826
2	6	0	-2.945595	3.335580	-0.179778
3	7	0	-2.629414	1.989324	-0.345121
4	6	0	-1.349284	1.725887	0.055934
5	7	0	-0.872311	2.943697	0.457183
6	79	0	-0.353549	-0.100162	0.107669
7	1	0	-1.642213	4.966488	0.563017
8	1	0	-3.902819	3.738654	-0.467293
9	6	0	-3.553513	1.023023	-0.863192
10	6	0	-3.171699	0.179686	-1.909454
11	6	0	-4.841631	0.959610	-0.326799
12	6	0	-4.091476	-0.741489	-2.410889
13	6	0	-5.756205	0.041457	-0.843425
14	6	0	-5.382585	-0.811541	-1.883336
15	1	0	-3.797073	-1.399811	-3.222447
16	1	0	-6.755825	-0.013157	-0.423327
17	1	0	-6.094378	-1.528742	-2.280575
18	6	0	0.442733	3.193985	0.974532
19	6	0	1.566562	2.692771	0.312887
20	6	0	0.579916	3.958935	2.135676
21	6	0	2.835648	2.949810	0.831898
22	6	0	1.854770	4.223742	2.636709
23	6	0	2.983116	3.716981	1.989250
24	1	0	3.704957	2.544514	0.323407
25	1	0	1.961814	4.814091	3.541683
26	1	0	3.973380	3.916879	2.387263
27	16	0	1.669985	-1.522378	-2.475803
28	6	0	3.241130	-0.963037	-1.844639
29	6	0	3.733106	0.259710	-2.331224
30	6	0	4.027856	-1.699389	-0.945787
31	6	0	4.984937	0.729434	-1.932592
32	1	0	3.130475	0.838799	-3.025609
33	6	0	5.269676	-1.212971	-0.535130
34	1	0	3.675539	-2.652589	-0.566557
35	6	0	5.757978	-0.000367	-1.026029
36	1	0	5.353514	1.671861	-2.329593
37	1	0	5.862345	-1.794044	0.166332
38	1	0	6.729292	0.368661	-0.710035
39	1	0	-0.302570	4.322219	2.653245
40	1	0	-5.115535	1.607921	0.499788
41	1	0	1.447905	2.100186	-0.586675
42	1	0	-2.168986	0.245872	-2.316137
43	6	0	0.110371	-2.873463	1.205241
44	6	0	0.681379	-3.049791	2.478809

45	6	0	-1.048785	-3.618616	0.914807
46	6	0	0.120398	-3.913526	3.420150
47	1	0	1.580328	-2.491792	2.732331
48	6	0	-1.605996	-4.492284	1.847667
49	1	0	-1.531480	-3.499886	-0.052095
50	6	0	-1.027287	-4.645031	3.110035
51	1	0	0.587508	-4.020931	4.396183
52	1	0	-2.501565	-5.052393	1.589393
53	1	0	-1.463568	-5.323113	3.838153
54	6	0	0.971794	-2.589668	-1.144553
55	1	0	0.038512	-2.926418	-1.605304
56	1	0	1.607357	-3.481185	-1.051507
57	6	0	0.727240	-1.912531	0.215210
58	1	0	1.706576	-1.622773	0.614115

P3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.580075	-1.687866	-1.057478
2	6	0	-1.617956	-0.320129	-0.534928
3	6	0	-1.322003	0.990798	-0.936318
4	6	0	-2.768312	-0.562271	0.230118
5	6	0	-2.159520	2.043340	-0.565315
6	1	0	-0.439565	1.176500	-1.538692
7	6	0	-3.604330	0.493452	0.596676
8	1	0	-3.005097	-1.579090	0.525973
9	6	0	-3.299910	1.797187	0.201546
10	1	0	-1.922817	3.055509	-0.880391
11	1	0	-4.494181	0.296219	1.187599
12	1	0	-3.952652	2.617804	0.484921
13	6	0	1.660759	-0.520211	0.220615
14	6	0	1.492041	0.562299	1.094257
15	6	0	2.694653	-0.454040	-0.726487
16	6	0	2.332448	1.675868	1.023363
17	1	0	0.703233	0.542130	1.838606
18	6	0	3.534169	0.654546	-0.799391
19	1	0	2.834992	-1.282315	-1.416624
20	6	0	3.355490	1.727255	0.078020
21	1	0	2.184503	2.503460	1.711339
22	1	0	4.330335	0.680663	-1.537952
23	1	0	4.010158	2.592241	0.025331
24	6	0	0.193688	-2.089500	1.635696

25	1	0	0.997744	-2.147606	2.377680
26	1	0	-0.528658	-1.342821	1.976571
27	1	0	-0.318131	-3.054090	1.598342
28	6	0	0.765038	-1.741299	0.260888
29	1	0	1.343821	-2.596509	-0.105495

P4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.397304	-1.974490	-0.450334
2	6	0	-2.408016	-0.518783	-0.150193
3	6	0	-2.688432	0.385204	-1.184904
4	6	0	-2.968621	-0.309543	1.116384
5	6	0	-3.501086	1.493158	-0.947289
6	1	0	-2.276915	0.211529	-2.174530
7	6	0	-3.795781	0.791959	1.345345
8	1	0	-2.753452	-1.011185	1.915789
9	6	0	-4.058941	1.697260	0.317055
10	1	0	-3.710560	2.189993	-1.753836
11	1	0	-4.227682	0.944583	2.330220
12	1	0	-4.698842	2.556020	0.497277
13	6	0	2.256934	-0.055962	0.370612
14	6	0	2.413320	1.278187	-0.029466
15	6	0	3.404039	-0.850602	0.500508
16	6	0	3.678438	1.804409	-0.292004
17	1	0	1.534523	1.911105	-0.129412
18	6	0	4.671306	-0.328741	0.239676
19	1	0	3.302163	-1.886440	0.815921
20	6	0	4.812481	1.001593	-0.158459
21	1	0	3.778864	2.842530	-0.596074
22	1	0	5.548534	-0.959695	0.351813
23	1	0	5.798452	1.410466	-0.359009
24	6	0	0.273533	-1.222695	-0.669791
25	1	0	0.220668	-0.464566	-1.456632
26	1	0	0.892620	-2.041688	-1.049474
27	6	0	0.879509	-0.636326	0.615394
28	1	0	0.208856	0.138702	1.001580
29	1	0	0.927529	-1.424228	1.374524

RC2

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.677504	-2.873952	0.285150
2	6	0	-0.676869	-2.874067	0.285160
3	7	0	-1.075582	-1.544552	0.177458
4	6	0	0.000132	-0.707078	0.099281
5	7	0	1.075994	-1.544369	0.177443
6	1	0	1.386775	-3.679248	0.384910
7	1	0	-1.386007	-3.679480	0.384922
8	6	0	-2.449162	-1.133111	0.121954
9	6	0	-2.905249	-0.101359	0.945628
10	6	0	-3.318851	-1.786328	-0.754773
11	6	0	-4.243337	0.286784	0.874738
12	1	0	-2.221504	0.388271	1.629883
13	6	0	-4.658131	-1.399858	-0.806111
14	1	0	-2.944368	-2.571081	-1.404716
15	6	0	-5.121267	-0.361424	0.004153
16	1	0	-4.596984	1.095031	1.506877
17	1	0	-5.334289	-1.902283	-1.490916
18	1	0	-6.162027	-0.056654	-0.044809
19	6	0	2.449506	-1.132697	0.121918
20	6	0	2.905478	-0.100961	0.945680
21	6	0	3.319270	-1.785724	-0.754876
22	6	0	4.243504	0.287390	0.874776
23	1	0	2.221702	0.388471	1.630045
24	6	0	4.658490	-1.399046	-0.806229
25	1	0	2.944891	-2.570494	-1.404857
26	6	0	5.121498	-0.360602	0.004095
27	1	0	4.597057	1.095621	1.506989
28	1	0	5.334702	-1.901323	-1.491089
29	1	0	6.162210	-0.055674	-0.044878
30	17	0	-0.001214	3.700342	-0.342063
31	47	0	0.000011	1.379099	-0.137763

1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.962066	3.031603	-1.664923
2	6	0	-2.149373	2.392284	-1.796354
3	7	0	-2.131782	1.330375	-0.896939
4	6	0	-0.962565	1.294359	-0.194555
5	7	0	-0.246311	2.344980	-0.688624

6	1	0	-0.548957	3.877589	-2.189574
7	1	0	-2.980991	2.568169	-2.458918
8	6	0	-3.221989	0.409906	-0.736447
9	6	0	-2.987516	-0.966554	-0.781670
10	6	0	-4.512067	0.913798	-0.553124
11	6	0	-4.062610	-1.842512	-0.625489
12	6	0	-5.579726	0.027410	-0.411863
13	6	0	-5.356494	-1.350588	-0.444074
14	1	0	-3.882548	-2.912484	-0.654209
15	1	0	-6.582614	0.415989	-0.263920
16	1	0	-6.188205	-2.038430	-0.326694
17	6	0	1.073605	2.717496	-0.264594
18	6	0	2.098427	1.768664	-0.261209
19	6	0	1.315638	4.038082	0.121651
20	6	0	3.375969	2.150856	0.149065
21	6	0	2.599955	4.410525	0.518458
22	6	0	3.630090	3.467821	0.536063
23	1	0	4.169582	1.411015	0.153109
24	1	0	2.790192	5.434526	0.824880
25	1	0	4.627330	3.759425	0.851081
26	16	0	0.367554	-3.477857	-0.452753
27	1	0	0.311174	-3.079938	0.843753
28	17	0	0.217289	-1.674388	2.907305
29	6	0	1.949804	-2.741596	-0.840350
30	6	0	2.812304	-2.257898	0.155047
31	6	0	2.343072	-2.677809	-2.185509
32	6	0	4.052148	-1.723024	-0.201850
33	1	0	2.512432	-2.294281	1.197745
34	6	0	3.584787	-2.143216	-2.529069
35	1	0	1.679433	-3.049944	-2.961221
36	6	0	4.447075	-1.663385	-1.540462
37	1	0	4.716058	-1.363436	0.580156
38	1	0	3.878124	-2.104149	-3.574634
39	1	0	5.416420	-1.254522	-1.810205
40	1	0	0.502385	4.757327	0.130301
41	1	0	1.905037	0.750014	-0.578945
42	1	0	-1.984093	-1.349471	-0.937553
43	1	0	-4.672152	1.986343	-0.500500
44	47	0	-0.415480	-0.056772	1.317058

TSc1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.001398	3.249399	-0.467241
2	6	0	-3.136809	2.513724	-0.534387
3	7	0	-2.754747	1.180472	-0.408439
4	6	0	-1.405026	1.063633	-0.251944
5	7	0	-0.952185	2.349492	-0.300868
6	1	0	-1.838736	4.311278	-0.553410
7	1	0	-4.162708	2.804628	-0.690845
8	6	0	-3.679964	0.084423	-0.407842
9	6	0	-3.456367	-1.017257	-1.236998
10	6	0	-4.803921	0.141232	0.419307
11	6	0	-4.363676	-2.076882	-1.222977
12	6	0	-5.711705	-0.917883	0.414721
13	6	0	-5.491827	-2.028828	-0.401739
14	1	0	-4.189405	-2.936853	-1.862047
15	1	0	-6.582197	-0.879075	1.062154
16	1	0	-6.195840	-2.855123	-0.396138
17	6	0	0.419846	2.743229	-0.150828
18	6	0	1.418510	2.088611	-0.875530
19	6	0	0.737808	3.782394	0.726644
20	6	0	2.750120	2.465703	-0.700009
21	6	0	2.070163	4.166063	0.878120
22	6	0	3.077243	3.506050	0.171437
23	1	0	3.527694	1.938278	-1.242997
24	1	0	2.320236	4.968829	1.564833
25	1	0	4.114381	3.798111	0.303997
26	16	0	1.197662	-2.721814	0.070325
27	1	0	1.076289	-2.276142	1.554994
28	17	0	0.616907	-1.390031	2.911499
29	6	0	2.792743	-1.986261	-0.328686
30	6	0	3.603977	-1.417637	0.663753
31	6	0	3.241788	-2.015327	-1.656844
32	6	0	4.846304	-0.881042	0.320967
33	1	0	3.256465	-1.384146	1.691427
34	6	0	4.484546	-1.474559	-1.989361
35	1	0	2.620087	-2.467038	-2.424614
36	6	0	5.292718	-0.904485	-1.002364
37	1	0	5.467838	-0.444452	1.098098
38	1	0	4.823553	-1.506897	-3.021438
39	1	0	6.263862	-0.492091	-1.261090
40	1	0	-0.044876	4.263859	1.304400
41	1	0	1.155824	1.293929	-1.564911
42	1	0	-2.585570	-1.038201	-1.882881
43	1	0	-4.950323	0.993196	1.075814

44	47	0	-0.252947	-0.683576	0.114466

2c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.116496	3.082194	0.417590
2	6	0	3.210547	2.284456	0.398346
3	7	0	2.750324	0.981642	0.225365
4	6	0	1.388931	0.942549	0.124718
5	7	0	1.012356	2.249308	0.255050
6	1	0	2.017222	4.145045	0.565615
7	1	0	4.256356	2.511913	0.525293
8	6	0	3.617249	-0.157597	0.134650
9	6	0	3.361455	-1.295641	0.903396
10	6	0	4.721642	-0.105355	-0.719452
11	6	0	4.214414	-2.394730	0.799354
12	6	0	5.576017	-1.204746	-0.804109
13	6	0	5.322155	-2.351547	-0.049322
14	1	0	4.012123	-3.282721	1.389839
15	1	0	6.431443	-1.167538	-1.471559
16	1	0	5.983862	-3.208918	-0.123808
17	6	0	-0.338031	2.729693	0.193639
18	6	0	-1.343725	2.094237	0.925687
19	6	0	-0.627694	3.841738	-0.601794
20	6	0	-2.653345	2.568341	0.842154
21	6	0	-1.936478	4.320179	-0.660985
22	6	0	-2.951123	3.682692	0.055838
23	1	0	-3.438018	2.059803	1.392422
24	1	0	-2.163270	5.181911	-1.281274
25	1	0	-3.970938	4.050408	-0.001808
26	16	0	-1.196819	-2.685074	-0.380513
27	6	0	-2.873840	-2.085681	-0.204777
28	6	0	-3.354253	-0.941956	-0.869562
29	6	0	-3.778568	-2.812668	0.590653
30	6	0	-4.681062	-0.533216	-0.728002
31	1	0	-2.679392	-0.379314	-1.508119
32	6	0	-5.106408	-2.406076	0.722857
33	1	0	-3.427584	-3.700584	1.107863
34	6	0	-5.567657	-1.260954	0.069311
35	1	0	-5.023916	0.355352	-1.253150
36	1	0	-5.783139	-2.987157	1.344770
37	1	0	-6.601765	-0.944880	0.174529

38	1	0	0.158394	4.311314	-1.184962
39	1	0	4.895089	0.777681	-1.326679
40	1	0	-1.104403	1.239529	1.548515
41	1	0	2.507585	-1.317455	1.571381
42	47	0	0.145540	-0.750539	-0.169887

TSc2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.286073	1.403073	0.567100
2	6	0	4.546939	0.095982	0.803312
3	7	0	3.434924	-0.619388	0.364331
4	6	0	2.479137	0.208961	-0.153286
5	7	0	3.019287	1.457299	-0.010662
6	1	0	4.856484	2.290903	0.786222
7	1	0	5.390976	-0.384638	1.270248
8	6	0	3.341326	-2.049469	0.432977
9	6	0	2.180840	-2.655126	0.921688
10	6	0	4.432311	-2.819498	0.019283
11	6	0	2.117100	-4.048214	0.980895
12	6	0	4.360952	-4.210128	0.099119
13	6	0	3.202951	-4.827121	0.576895
14	1	0	1.212139	-4.517487	1.353809
15	1	0	5.206806	-4.809046	-0.224819
16	1	0	3.147375	-5.910142	0.631980
17	6	0	2.393725	2.677546	-0.426965
18	6	0	1.076562	2.955444	-0.052391
19	6	0	3.124367	3.587850	-1.195620
20	6	0	0.488145	4.151241	-0.466458
21	6	0	2.529794	4.785606	-1.592383
22	6	0	1.210510	5.068024	-1.232341
23	1	0	-0.535130	4.366011	-0.174600
24	1	0	3.095950	5.491270	-2.192775
25	1	0	0.748641	5.999166	-1.546232
26	16	0	-1.472493	-1.214204	0.801388
27	6	0	-2.035621	0.034894	1.919703
28	6	0	-3.408414	0.164228	2.220204
29	6	0	-1.144909	0.936152	2.541607
30	6	0	-3.864635	1.157843	3.085616
31	1	0	-4.111811	-0.529876	1.771384
32	6	0	-1.604680	1.919583	3.416675
33	1	0	-0.080379	0.838096	2.346190

34	6	0	-2.969450	2.044133	3.690541
35	1	0	-4.928901	1.233960	3.296341
36	1	0	-0.891930	2.592200	3.888801
37	1	0	-3.327643	2.812461	4.369865
38	1	0	4.139803	3.348802	-1.496319
39	1	0	5.318071	-2.334762	-0.379871
40	1	0	0.523475	2.255746	0.564315
41	1	0	1.334963	-2.054783	1.242024
42	6	0	-1.118070	-0.560804	-2.329716
43	1	0	-0.949793	-0.436492	-3.395022
44	6	0	-2.230418	-0.730487	-1.750883
45	6	0	-3.632163	-0.837760	-1.505241
46	6	0	-4.401936	0.320255	-1.267476
47	6	0	-4.280219	-2.089633	-1.583647
48	6	0	-5.782290	0.223572	-1.112057
49	1	0	-3.903167	1.281088	-1.201100
50	6	0	-5.658685	-2.173601	-1.431392
51	1	0	-3.685205	-2.980454	-1.754178
52	6	0	-6.414342	-1.019528	-1.193236
53	1	0	-6.366248	1.120307	-0.926422
54	1	0	-6.149254	-3.140566	-1.494762
55	1	0	-7.491209	-1.091238	-1.070667
56	47	0	0.563340	-0.301207	-0.954414

TSc3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.871347	-1.924772	2.927148
2	6	0	3.030532	-1.636071	2.289435
3	7	0	2.693372	-0.867258	1.177679
4	6	0	1.344999	-0.656626	1.107836
5	7	0	0.852061	-1.326518	2.190607
6	1	0	1.672097	-2.521039	3.802609
7	1	0	4.045973	-1.931900	2.496360
8	6	0	3.657081	-0.358913	0.245101
9	6	0	3.437854	-0.488718	-1.129128
10	6	0	4.818093	0.248332	0.731854
11	6	0	4.391555	0.011053	-2.017289
12	6	0	5.770024	0.729387	-0.167161
13	6	0	5.557448	0.614859	-1.542403
14	1	0	4.219275	-0.084136	-3.084820
15	1	0	6.670741	1.204233	0.209962

16	1	0	6.296947	0.995600	-2.240330
17	6	0	-0.535029	-1.404409	2.548331
18	6	0	-1.476197	-1.824920	1.605853
19	6	0	-0.920650	-1.073454	3.850103
20	6	0	-2.820786	-1.898447	1.973760
21	6	0	-2.265292	-1.163286	4.209480
22	6	0	-3.216750	-1.571671	3.271885
23	1	0	-3.547189	-2.223641	1.236264
24	1	0	-2.568635	-0.902296	5.218878
25	1	0	-4.263481	-1.635232	3.553671
26	16	0	-0.142975	-0.729388	-2.902924
27	6	0	-1.423488	-1.861054	-2.404504
28	6	0	-1.104148	-3.201607	-2.103814
29	6	0	-2.774116	-1.472454	-2.308355
30	6	0	-2.092751	-4.111000	-1.727615
31	1	0	-0.070055	-3.525313	-2.181964
32	6	0	-3.759290	-2.384719	-1.927068
33	1	0	-3.047701	-0.446813	-2.534223
34	6	0	-3.428920	-3.710515	-1.633321
35	1	0	-1.816812	-5.140118	-1.510204
36	1	0	-4.794508	-2.056476	-1.868135
37	1	0	-4.198774	-4.421066	-1.346116
38	1	0	-0.177575	-0.731066	4.563988
39	1	0	4.963486	0.360515	1.801954
40	1	0	-1.166471	-2.105172	0.604912
41	1	0	2.535676	-0.964626	-1.501525
42	6	0	-1.060225	1.613685	-2.399260
43	1	0	-1.238260	1.610391	-3.453028
44	6	0	-0.970894	2.104935	-1.242337
45	6	0	-1.379328	3.285173	-0.484867
46	6	0	-0.592650	3.794598	0.563477
47	6	0	-2.586753	3.942550	-0.796038
48	6	0	-0.984505	4.937973	1.257777
49	1	0	0.329698	3.283143	0.822419
50	6	0	-2.986484	5.070166	-0.082991
51	1	0	-3.207647	3.553370	-1.597144
52	6	0	-2.184890	5.577980	0.942807
53	1	0	-0.356169	5.322039	2.056708
54	1	0	-3.923866	5.558951	-0.334435
55	1	0	-2.496444	6.460329	1.494349
56	47	0	0.249245	0.430609	-0.355181

3c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.100035	2.383647	0.204809
2	6	0	4.831712	1.258215	0.382459
3	7	0	3.955373	0.187164	0.227694
4	6	0	2.687524	0.612791	-0.053635
5	7	0	2.794850	1.974673	-0.055693
6	1	0	4.372900	3.423884	0.273929
7	1	0	5.869659	1.119764	0.637430
8	6	0	4.360808	-1.183924	0.332165
9	6	0	3.629750	-2.072909	1.123942
10	6	0	5.502215	-1.610099	-0.351811
11	6	0	4.042265	-3.402453	1.215984
12	6	0	5.913278	-2.938538	-0.241350
13	6	0	5.183176	-3.837228	0.538780
14	1	0	3.471161	-4.095439	1.825832
15	1	0	6.797429	-3.271559	-0.776285
16	1	0	5.501401	-4.872205	0.617593
17	6	0	1.722884	2.891842	-0.324113
18	6	0	0.485938	2.734980	0.305855
19	6	0	1.944080	3.947498	-1.213031
20	6	0	-0.541404	3.638566	0.028825
21	6	0	0.915904	4.854441	-1.469514
22	6	0	-0.327035	4.699906	-0.852511
23	1	0	-1.506603	3.507114	0.506719
24	1	0	1.085227	5.672915	-2.162721
25	1	0	-1.128573	5.401949	-1.061026
26	16	0	-1.977733	-0.448805	1.420149
27	6	0	-3.107164	0.877630	1.017077
28	6	0	-3.539341	1.153030	-0.287971
29	6	0	-3.525139	1.712689	2.066942
30	6	0	-4.377773	2.242200	-0.531726
31	1	0	-3.217258	0.518631	-1.105986
32	6	0	-4.350412	2.807297	1.811459
33	1	0	-3.205926	1.499036	3.083693
34	6	0	-4.784294	3.077741	0.510471
35	1	0	-4.709974	2.439026	-1.547708
36	1	0	-4.665058	3.443319	2.634771
37	1	0	-5.435602	3.924490	0.314290
38	1	0	2.902135	4.043485	-1.714697
39	1	0	6.048134	-0.913153	-0.980197
40	1	0	0.322922	1.914148	0.995441
41	1	0	2.752322	-1.724958	1.657296

42	6	0	-0.807142	-1.656265	-0.722797
43	1	0	-0.856024	-2.430280	-1.496588
44	6	0	-1.968385	-1.522263	-0.041843
45	6	0	-3.223359	-2.276065	-0.335529
46	6	0	-3.548147	-2.599543	-1.666880
47	6	0	-4.103676	-2.702821	0.674212
48	6	0	-4.688873	-3.339270	-1.973085
49	1	0	-2.900671	-2.251694	-2.466324
50	6	0	-5.244497	-3.443968	0.368172
51	1	0	-3.882252	-2.454160	1.706898
52	6	0	-5.544099	-3.768584	-0.956059
53	1	0	-4.916543	-3.570146	-3.010552
54	1	0	-5.902508	-3.769050	1.169876
55	1	0	-6.437119	-4.339973	-1.193596
56	47	0	0.940426	-0.561668	-0.408303

4c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.662859	-4.065230	0.334743
2	6	0	2.862660	-3.582840	-0.067391
3	7	0	2.699699	-2.211340	-0.243437
4	6	0	1.424732	-1.816342	0.049023
5	7	0	0.795540	-2.977696	0.396683
6	1	0	1.338787	-5.071167	0.545594
7	1	0	3.793856	-4.083053	-0.277642
8	6	0	3.758258	-1.336701	-0.656088
9	6	0	3.548812	-0.424083	-1.692817
10	6	0	4.998948	-1.421673	-0.019307
11	6	0	4.590538	0.418964	-2.080549
12	6	0	6.037659	-0.583633	-0.425039
13	6	0	5.834834	0.339872	-1.452268
14	1	0	4.426627	1.133686	-2.880882
15	1	0	7.000568	-0.645147	0.072719
16	1	0	6.642563	0.996477	-1.760507
17	6	0	-0.575212	-3.087071	0.810186
18	6	0	-1.583977	-2.453745	0.080311
19	6	0	-0.880789	-3.845916	1.943403
20	6	0	-2.909375	-2.573624	0.501522
21	6	0	-2.210371	-3.972926	2.345367
22	6	0	-3.224692	-3.335611	1.628106
23	1	0	-3.690695	-2.069256	-0.057442

24	1	0	-2.448679	-4.559239	3.227704
25	1	0	-4.257930	-3.428318	1.948414
26	16	0	-2.047161	1.126353	-1.932465
27	6	0	-3.681058	0.805274	-1.277839
28	6	0	-4.596105	0.131624	-2.104292
29	6	0	-4.064556	1.156900	0.024149
30	6	0	-5.866561	-0.192112	-1.629910
31	1	0	-4.311545	-0.131868	-3.119663
32	6	0	-5.344259	0.841690	0.484738
33	1	0	-3.357857	1.667122	0.670249
34	6	0	-6.249905	0.163382	-0.333217
35	1	0	-6.563529	-0.713529	-2.280824
36	1	0	-5.629769	1.124277	1.494744
37	1	0	-7.243408	-0.081014	0.031298
38	1	0	-0.084590	-4.311662	2.516023
39	1	0	5.140532	-2.120443	0.799411
40	1	0	-1.338770	-1.866833	-0.797865
41	1	0	2.583881	-0.378094	-2.185091
42	6	0	-1.353350	2.324379	-0.804877
43	1	0	-1.871456	3.286528	-0.818029
44	6	0	-0.241027	2.088175	-0.076124
45	6	0	0.338980	3.228537	0.676218
46	6	0	0.865467	3.037323	1.969064
47	6	0	0.400865	4.530016	0.137456
48	6	0	1.391096	4.098255	2.703978
49	1	0	0.848232	2.036537	2.393788
50	6	0	0.942695	5.589908	0.864705
51	1	0	0.038724	4.699639	-0.872431
52	6	0	1.434818	5.382509	2.154766
53	1	0	1.777520	3.921211	3.704586
54	1	0	0.984530	6.581044	0.419714
55	1	0	1.858483	6.207773	2.720456
56	47	0	0.612339	0.158194	-0.003738

RC3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.677191	-2.634703	0.348357
2	6	0	-0.677110	-2.634714	0.348368
3	7	0	-1.077141	-1.311044	0.191172
4	6	0	0.000021	-0.474276	0.082691
5	7	0	1.077197	-1.311023	0.191174

6	1	0	1.384804	-3.436523	0.481101
7	1	0	-1.384707	-3.436547	0.481116
8	6	0	-2.448503	-0.899844	0.117653
9	6	0	-2.889797	0.205164	0.849676
10	6	0	-3.333861	-1.624207	-0.685013
11	6	0	-4.227089	0.591801	0.761634
12	1	0	-2.195195	0.753000	1.476602
13	6	0	-4.672348	-1.237906	-0.752336
14	1	0	-2.972411	-2.464900	-1.269038
15	6	0	-5.120581	-0.128448	-0.033235
16	1	0	-4.567943	1.456224	1.322507
17	1	0	-5.359512	-1.796990	-1.379987
18	1	0	-6.160937	0.175547	-0.094756
19	6	0	2.448552	-0.899797	0.117653
20	6	0	2.889814	0.205255	0.849629
21	6	0	3.333935	-1.624175	-0.684972
22	6	0	4.227099	0.591917	0.761584
23	1	0	2.195195	0.753108	1.476520
24	6	0	4.672415	-1.237848	-0.752299
25	1	0	2.972512	-2.464900	-1.268968
26	6	0	5.120617	-0.128349	-0.033242
27	1	0	4.567927	1.456372	1.322422
28	1	0	5.359596	-1.796945	-1.379919
29	1	0	6.160967	0.175666	-0.094764
30	17	0	-0.000128	3.519558	-0.384161
31	29	0	-0.000022	1.404471	-0.172255

1d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.261251	2.859247	-1.628080
2	6	0	-2.402427	2.136242	-1.731467
3	7	0	-2.307494	1.105752	-0.801828
4	6	0	-1.133282	1.170494	-0.104986
5	7	0	-0.493813	2.254701	-0.637441
6	1	0	-0.910295	3.713687	-2.183186
7	1	0	-3.246477	2.234396	-2.394336
8	6	0	-3.324416	0.113522	-0.605508
9	6	0	-2.981668	-1.240771	-0.588276
10	6	0	-4.651850	0.520375	-0.450143
11	6	0	-3.984388	-2.191851	-0.396492
12	6	0	-5.646646	-0.441305	-0.273815

13	6	0	-5.314646	-1.797112	-0.242460
14	1	0	-3.720553	-3.244544	-0.376947
15	1	0	-6.678302	-0.127627	-0.147242
16	1	0	-6.089925	-2.543106	-0.097184
17	6	0	0.800805	2.724566	-0.237441
18	6	0	1.871999	1.831681	-0.158476
19	6	0	0.975526	4.081177	0.047698
20	6	0	3.126813	2.306866	0.222823
21	6	0	2.237906	4.546397	0.415822
22	6	0	3.313757	3.660899	0.506719
23	1	0	3.955963	1.609504	0.283103
24	1	0	2.375161	5.599147	0.643094
25	1	0	4.293884	4.025561	0.798556
26	16	0	0.671033	-3.327763	-0.333512
27	1	0	0.467923	-2.817757	0.906831
28	17	0	0.082622	-1.300709	2.851969
29	6	0	2.288425	-2.615291	-0.602468
30	6	0	3.009845	-1.987982	0.424650
31	6	0	2.854958	-2.716913	-1.881729
32	6	0	4.282457	-1.474646	0.164237
33	1	0	2.578503	-1.901463	1.417192
34	6	0	4.127247	-2.201968	-2.128407
35	1	0	2.301143	-3.200737	-2.681561
36	6	0	4.848761	-1.577951	-1.108336
37	1	0	4.836559	-1.003069	0.971870
38	1	0	4.554980	-2.290696	-3.123351
39	1	0	5.841760	-1.183052	-1.301875
40	1	0	0.127817	4.757987	0.002609
41	1	0	1.730858	0.783764	-0.398962
42	1	0	-1.949647	-1.545529	-0.729972
43	1	0	-4.897309	1.577946	-0.444466
44	29	0	-0.563157	0.039814	1.307595

TSd1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.715360	3.188249	-0.581814
2	6	0	-2.887340	2.511906	-0.636933
3	7	0	-2.580678	1.167246	-0.446200
4	6	0	-1.239438	0.983905	-0.259130
5	7	0	-0.718143	2.243190	-0.357053
6	1	0	-1.495219	4.234763	-0.714440

7	1	0	-3.892885	2.850227	-0.826138
8	6	0	-3.561474	0.122977	-0.414022
9	6	0	-3.364764	-1.042080	-1.159637
10	6	0	-4.714212	0.291412	0.356721
11	6	0	-4.327755	-2.050302	-1.117587
12	6	0	-5.677636	-0.717099	0.379068
13	6	0	-5.485368	-1.889737	-0.353514
14	1	0	-4.173458	-2.958792	-1.691393
15	1	0	-6.570632	-0.590238	0.983237
16	1	0	-6.233001	-2.676406	-0.326844
17	6	0	0.669433	2.569033	-0.202870
18	6	0	1.642849	1.806738	-0.852686
19	6	0	1.030376	3.655516	0.597792
20	6	0	2.989693	2.126514	-0.681410
21	6	0	2.378843	3.979162	0.745519
22	6	0	3.359630	3.214222	0.111558
23	1	0	3.744764	1.517630	-1.167815
24	1	0	2.661034	4.818991	1.373040
25	1	0	4.408893	3.461616	0.240229
26	16	0	0.789031	-2.650636	0.159799
27	1	0	0.677820	-2.086063	1.627380
28	17	0	0.262852	-1.061276	2.854576
29	6	0	2.463785	-2.121060	-0.241466
30	6	0	3.359276	-1.717168	0.758889
31	6	0	2.889811	-2.156179	-1.577107
32	6	0	4.662503	-1.350621	0.418537
33	1	0	3.031934	-1.678469	1.792615
34	6	0	4.194770	-1.787940	-1.907784
35	1	0	2.201012	-2.479153	-2.352459
36	6	0	5.087425	-1.383938	-0.911660
37	1	0	5.348340	-1.039912	1.201981
38	1	0	4.514836	-1.824863	-2.945722
39	1	0	6.105495	-1.105814	-1.168997
40	1	0	0.266505	4.221010	1.122013
41	1	0	1.349339	0.973393	-1.481316
42	1	0	-2.470752	-1.150459	-1.763667
43	1	0	-4.840771	1.190138	0.952097
44	29	0	-0.316026	-0.637925	0.167642

2d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.643947	3.042868	0.590136
2	6	0	2.819545	2.371265	0.616625
3	7	0	2.530787	1.047861	0.295422
4	6	0	1.194862	0.872443	0.056817
5	7	0	0.661086	2.117507	0.251210
6	1	0	1.412691	4.071038	0.814863
7	1	0	3.815415	2.697634	0.867719
8	6	0	3.524365	0.019425	0.201694
9	6	0	3.300252	-1.228498	0.788854
10	6	0	4.720376	0.286789	-0.469951
11	6	0	4.279664	-2.216480	0.687316
12	6	0	5.699118	-0.703749	-0.551140
13	6	0	5.480176	-1.957047	0.023395
14	1	0	4.101661	-3.188646	1.136115
15	1	0	6.626361	-0.497540	-1.076942
16	1	0	6.240253	-2.728867	-0.048440
17	6	0	-0.723439	2.451620	0.084015
18	6	0	-1.715357	1.604396	0.582984
19	6	0	-1.063983	3.631145	-0.584495
20	6	0	-3.057686	1.932031	0.390802
21	6	0	-2.408859	3.961416	-0.750324
22	6	0	-3.406817	3.111652	-0.269036
23	1	0	-3.822038	1.255062	0.758574
24	1	0	-2.673737	4.875515	-1.273081
25	1	0	-4.452570	3.365718	-0.412695
26	16	0	-0.810417	-2.565241	-0.868796
27	6	0	-2.437415	-2.169846	-0.217527
28	6	0	-3.526094	-1.998960	-1.090567
29	6	0	-2.678586	-2.077236	1.165811
30	6	0	-4.804758	-1.731980	-0.599099
31	1	0	-3.357668	-2.075316	-2.160291
32	6	0	-3.957248	-1.802634	1.655284
33	1	0	-1.853908	-2.233584	1.855136
34	6	0	-5.029506	-1.626955	0.776047
35	1	0	-5.629713	-1.604959	-1.295912
36	1	0	-4.117467	-1.738380	2.729011
37	1	0	-6.026419	-1.423843	1.157447
38	1	0	-0.286659	4.268339	-0.994635
39	1	0	4.872002	1.251725	-0.943663
40	1	0	-1.446513	0.696255	1.110611
41	1	0	2.371342	-1.420836	1.314076
42	29	0	0.266730	-0.734932	-0.413428

TSd2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.407145	1.093757	0.383573
2	6	0	4.562340	-0.223668	0.649633
3	7	0	3.345749	-0.836662	0.356555
4	6	0	2.422665	0.067325	-0.103381
5	7	0	3.098593	1.258936	-0.067146
6	1	0	5.080346	1.925693	0.510310
7	1	0	5.398498	-0.770213	1.054035
8	6	0	3.107310	-2.239014	0.512817
9	6	0	1.939045	-2.681817	1.139737
10	6	0	4.059871	-3.151334	0.049910
11	6	0	1.725347	-4.052693	1.288501
12	6	0	3.840916	-4.518630	0.218312
13	6	0	2.672887	-4.972240	0.834249
14	1	0	0.816813	-4.396496	1.773194
15	1	0	4.579214	-5.227714	-0.144061
16	1	0	2.502472	-6.037343	0.959262
17	6	0	2.545871	2.523537	-0.442514
18	6	0	1.280566	2.895814	0.018701
19	6	0	3.292064	3.384727	-1.252308
20	6	0	0.760851	4.138757	-0.343870
21	6	0	2.767290	4.630041	-1.597647
22	6	0	1.501332	5.008961	-1.146378
23	1	0	-0.222802	4.421151	0.017652
24	1	0	3.345323	5.297871	-2.229414
25	1	0	1.094351	5.977887	-1.419658
26	16	0	-1.273576	-0.579500	1.050211
27	6	0	-2.136459	0.925814	1.421609
28	6	0	-2.232469	1.989689	0.500333
29	6	0	-2.781713	1.077665	2.665356
30	6	0	-2.940106	3.151817	0.813681
31	1	0	-1.751251	1.895321	-0.468522
32	6	0	-3.477957	2.244469	2.977934
33	1	0	-2.729044	0.265571	3.384138
34	6	0	-3.564155	3.290778	2.055748
35	1	0	-3.007675	3.951109	0.078618
36	1	0	-3.961768	2.334062	3.947526
37	1	0	-4.112123	4.196529	2.299284
38	1	0	4.263226	3.072721	-1.624037
39	1	0	4.951457	-2.793333	-0.455740
40	1	0	0.715754	2.225622	0.657934

41	1	0	1.212828	-1.964052	1.507848
42	6	0	-0.709990	-0.823955	-2.079059
43	1	0	-0.532883	-0.926898	-3.146344
44	6	0	-1.812298	-1.047316	-1.486440
45	6	0	-3.178865	-1.420312	-1.280998
46	6	0	-4.204419	-0.453247	-1.331073
47	6	0	-3.522679	-2.779288	-1.118052
48	6	0	-5.536089	-0.841276	-1.214230
49	1	0	-3.942136	0.591995	-1.447584
50	6	0	-4.856251	-3.156012	-1.009005
51	1	0	-2.731719	-3.520807	-1.075291
52	6	0	-5.866458	-2.189289	-1.054014
53	1	0	-6.319340	-0.089720	-1.249288
54	1	0	-5.111799	-4.204578	-0.886434
55	1	0	-6.907290	-2.486907	-0.964563
56	29	0	0.629063	-0.298613	-0.701202

TSd3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.778906	-1.827597	2.952625
2	6	0	2.947602	-1.684444	2.285395
3	7	0	2.644991	-1.054073	1.080441
4	6	0	1.305044	-0.784813	0.976600
5	7	0	0.785881	-1.280883	2.143063
6	1	0	1.556031	-2.296102	3.897162
7	1	0	3.947020	-2.003560	2.531775
8	6	0	3.627133	-0.717614	0.094315
9	6	0	3.391326	-1.004664	-1.253020
10	6	0	4.824038	-0.119420	0.498403
11	6	0	4.362773	-0.675083	-2.198802
12	6	0	5.793326	0.191550	-0.455376
13	6	0	5.564089	-0.082058	-1.804997
14	1	0	4.178816	-0.894635	-3.245970
15	1	0	6.721540	0.659804	-0.142071
16	1	0	6.317538	0.166914	-2.546072
17	6	0	-0.595121	-1.218131	2.517143
18	6	0	-1.584900	-1.577583	1.599929
19	6	0	-0.934756	-0.804669	3.808622
20	6	0	-2.926074	-1.507976	1.979076
21	6	0	-2.277545	-0.753404	4.181679
22	6	0	-3.274900	-1.100607	3.267821

23	1	0	-3.689895	-1.780477	1.257790
24	1	0	-2.542343	-0.427629	5.183116
25	1	0	-4.319674	-1.051491	3.559464
26	16	0	-0.235905	-0.925696	-2.633632
27	6	0	-1.882901	-1.495974	-2.243163
28	6	0	-2.082575	-2.855719	-1.939763
29	6	0	-3.001345	-0.645226	-2.268115
30	6	0	-3.362239	-3.348577	-1.680595
31	1	0	-1.227710	-3.525754	-1.921294
32	6	0	-4.276912	-1.141603	-1.997413
33	1	0	-2.864104	0.405775	-2.495525
34	6	0	-4.468048	-2.494445	-1.704756
35	1	0	-3.493732	-4.404808	-1.459621
36	1	0	-5.127695	-0.465432	-2.023510
37	1	0	-5.464329	-2.879091	-1.505832
38	1	0	-0.157167	-0.504143	4.504190
39	1	0	4.983881	0.119400	1.545314
40	1	0	-1.314952	-1.915800	0.606227
41	1	0	2.462076	-1.477762	-1.553179
42	6	0	-0.329749	1.376566	-2.201924
43	1	0	-0.143403	1.595261	-3.239180
44	6	0	-0.498695	1.846763	-1.024445
45	6	0	-0.776497	3.134991	-0.406551
46	6	0	-0.224027	3.480134	0.840794
47	6	0	-1.624447	4.067596	-1.039688
48	6	0	-0.481359	4.722583	1.416813
49	1	0	0.411670	2.758663	1.345515
50	6	0	-1.901052	5.297158	-0.447085
51	1	0	-2.069442	3.810888	-1.996698
52	6	0	-1.325391	5.635871	0.780512
53	1	0	-0.033177	4.973359	2.374729
54	1	0	-2.562329	5.998146	-0.949831
55	1	0	-1.538318	6.597531	1.238610
56	29	0	0.383926	0.145349	-0.434335

3d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.054978	2.296987	0.217466
2	6	0	4.737370	1.151470	0.454071
3	7	0	3.843180	0.105562	0.243981
4	6	0	2.609935	0.566536	-0.130574

5	7	0	2.759965	1.926310	-0.133517
6	1	0	4.354675	3.328499	0.302698
7	1	0	5.749301	0.985733	0.785588
8	6	0	4.190599	-1.276444	0.390383
9	6	0	3.346193	-2.139479	1.093849
10	6	0	5.385476	-1.743026	-0.163956
11	6	0	3.700222	-3.482108	1.227253
12	6	0	5.736336	-3.084493	-0.011281
13	6	0	4.894036	-3.956777	0.680563
14	1	0	3.041207	-4.154075	1.768075
15	1	0	6.662505	-3.448115	-0.445844
16	1	0	5.166058	-5.001917	0.791852
17	6	0	1.732371	2.867189	-0.474762
18	6	0	0.438691	2.707019	0.027946
19	6	0	2.049020	3.947992	-1.302794
20	6	0	-0.545950	3.635129	-0.314217
21	6	0	1.060881	4.878189	-1.624504
22	6	0	-0.236876	4.722414	-1.133811
23	1	0	-1.553330	3.501027	0.066198
24	1	0	1.305310	5.716081	-2.270520
25	1	0	-1.005759	5.444229	-1.392258
26	16	0	-1.671319	-0.556927	1.359486
27	6	0	-2.920346	0.715870	1.209524
28	6	0	-3.480454	1.106611	-0.015159
29	6	0	-3.310586	1.381037	2.383703
30	6	0	-4.417418	2.141250	-0.056886
31	1	0	-3.186364	0.600914	-0.927955
32	6	0	-4.235715	2.422231	2.330197
33	1	0	-2.890085	1.077165	3.338755
34	6	0	-4.797272	2.807759	1.109833
35	1	0	-4.850096	2.427000	-1.012183
36	1	0	-4.526008	2.927114	3.247806
37	1	0	-5.525814	3.612320	1.070786
38	1	0	3.050747	4.045984	-1.709738
39	1	0	6.020744	-1.067250	-0.728191
40	1	0	0.201414	1.868316	0.673969
41	1	0	2.427605	-1.761282	1.528541
42	6	0	-0.546424	-1.459980	-0.937835
43	1	0	-0.593209	-2.146274	-1.792336
44	6	0	-1.695210	-1.448516	-0.219557
45	6	0	-2.933503	-2.208646	-0.557808
46	6	0	-3.269288	-2.429865	-1.907702
47	6	0	-3.791072	-2.737299	0.422905
48	6	0	-4.396059	-3.169836	-2.260174

49	1	0	-2.641742	-2.002131	-2.683751
50	6	0	-4.918791	-3.477961	0.070329
51	1	0	-3.561515	-2.569594	1.469978
52	6	0	-5.228129	-3.701312	-1.272313
53	1	0	-4.631651	-3.321083	-3.310485
54	1	0	-5.558790	-3.881933	0.850441
55	1	0	-6.110626	-4.272871	-1.545941
56	29	0	1.030911	-0.462475	-0.552023

4d

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.816334	-3.872746	0.294731
2	6	0	2.940634	-3.349205	-0.249289
3	7	0	2.714217	-1.983309	-0.392655
4	6	0	1.471643	-1.630489	0.058883
5	7	0	0.928445	-2.815785	0.473468
6	1	0	1.554154	-4.890611	0.532106
7	1	0	3.852583	-3.819181	-0.579228
8	6	0	3.680144	-1.069815	-0.926404
9	6	0	3.296624	-0.125955	-1.882754
10	6	0	5.005316	-1.144508	-0.489452
11	6	0	4.249818	0.756746	-2.390751
12	6	0	5.952880	-0.266549	-1.015875
13	6	0	5.577184	0.687209	-1.963506
14	1	0	3.950917	1.494816	-3.128427
15	1	0	6.981511	-0.320925	-0.672711
16	1	0	6.315052	1.374652	-2.365514
17	6	0	-0.375360	-2.964577	1.052736
18	6	0	-1.472931	-2.307714	0.490425
19	6	0	-0.529442	-3.779821	2.177752
20	6	0	-2.731619	-2.462215	1.073464
21	6	0	-1.795331	-3.940445	2.740810
22	6	0	-2.896740	-3.280317	2.192735
23	1	0	-3.579631	-1.938585	0.643858
24	1	0	-1.914791	-4.570781	3.616867
25	1	0	-3.879552	-3.400674	2.638332
26	16	0	-1.804888	0.949958	-1.923547
27	6	0	-3.534513	0.698914	-1.538007
28	6	0	-4.358492	0.153549	-2.535981
29	6	0	-4.083228	0.991564	-0.280941
30	6	0	-5.703695	-0.101522	-2.275638

31	1	0	-3.943670	-0.062995	-3.516828
32	6	0	-5.436017	0.746390	-0.034572
33	1	0	-3.450132	1.407450	0.496151
34	6	0	-6.251995	0.196255	-1.025029
35	1	0	-6.328748	-0.524500	-3.057644
36	1	0	-5.850482	0.984900	0.941610
37	1	0	-7.302938	0.006060	-0.827784
38	1	0	0.335536	-4.262698	2.621909
39	1	0	5.284810	-1.866204	0.271871
40	1	0	-1.348205	-1.681612	-0.386990
41	1	0	2.267434	-0.087988	-2.222161
42	6	0	-1.248785	2.103733	-0.680178
43	1	0	-1.802398	3.046165	-0.680222
44	6	0	-0.179138	1.855074	0.108562
45	6	0	0.306134	2.967419	0.965396
46	6	0	0.753103	2.709506	2.276521
47	6	0	0.354090	4.302591	0.515534
48	6	0	1.189332	3.736853	3.111006
49	1	0	0.741210	1.683671	2.636967
50	6	0	0.804626	5.330464	1.344030
51	1	0	0.053906	4.525433	-0.504360
52	6	0	1.218801	5.055287	2.648681
53	1	0	1.515186	3.507981	4.122639
54	1	0	0.837041	6.349844	0.967209
55	1	0	1.571310	5.855651	3.293495
56	29	0	0.669077	0.124497	0.096296
