Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2017

RSC Advances

Electronic Supplementary Information (ESI)

A comparative study of inter- and intramolecular C-H aminations: mechanism and site selectivity

Juping Wang,*[a] Kangcheng Zheng,[b] Binbin Lin[a] and Yuping Weng[a]

[a] School of Pharmacy, Guangdong Pharmaceutical University, Guangzhou, 510006, P. R. China
[b] School of Chemistry and Chemical Engineering, Sun Yat-sen University, Guangzhou, 510275, P. R. China

Table of contents

1. Two parts of intramolecular C-H amintaion process.....S2
2. Important frontier orbital diagrams of Rh_2-nitrene.....S3
3. Mechanisms of intramolecular C-H aminations.....S4
4. Optimized structures and geometrical parameters for intermolecular aminations.....S5
5. Surface plots and values of the spin density distribution of triplet species.....S6
6. Calculated NBO charge (in e) for selected atoms in inter- and intramolecular aminations.....S7
7. Cartesian coordinates for the calculated structures.....S8

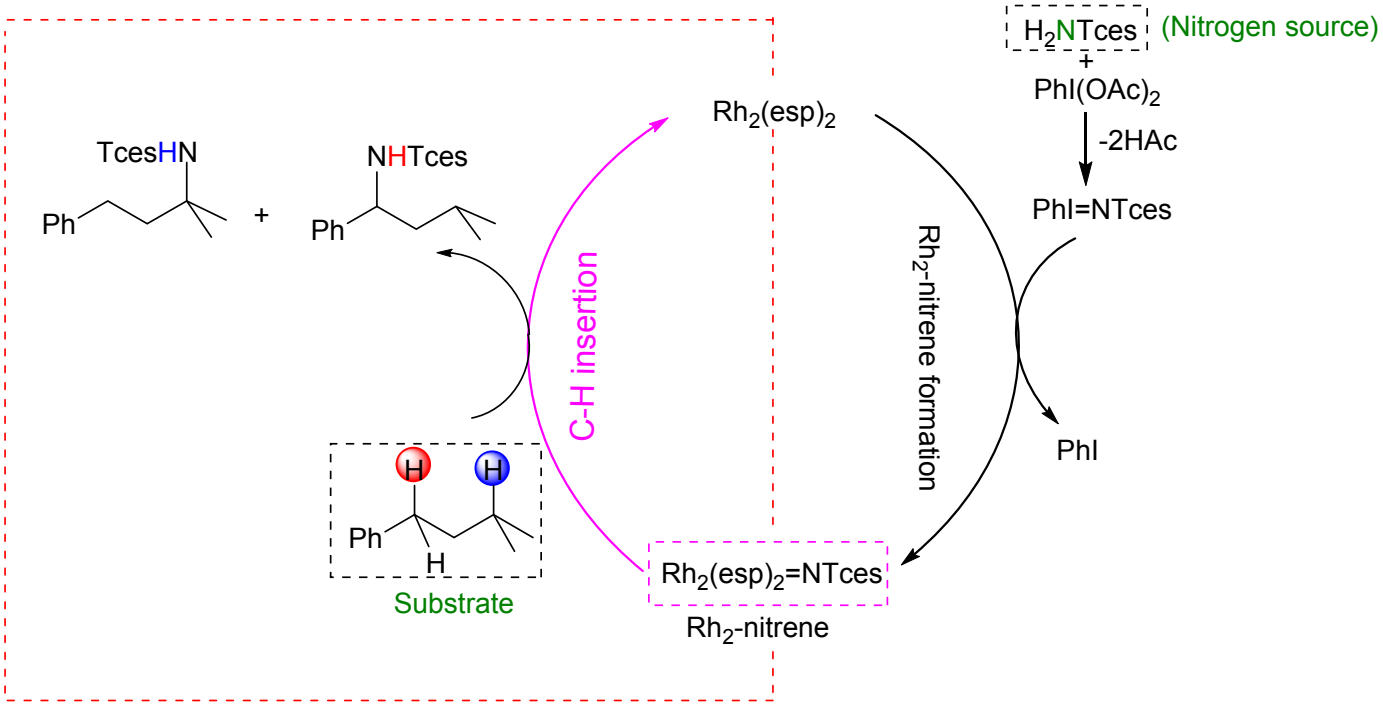

Fig. S1 Two parts of intermolecular C-H amintaion process

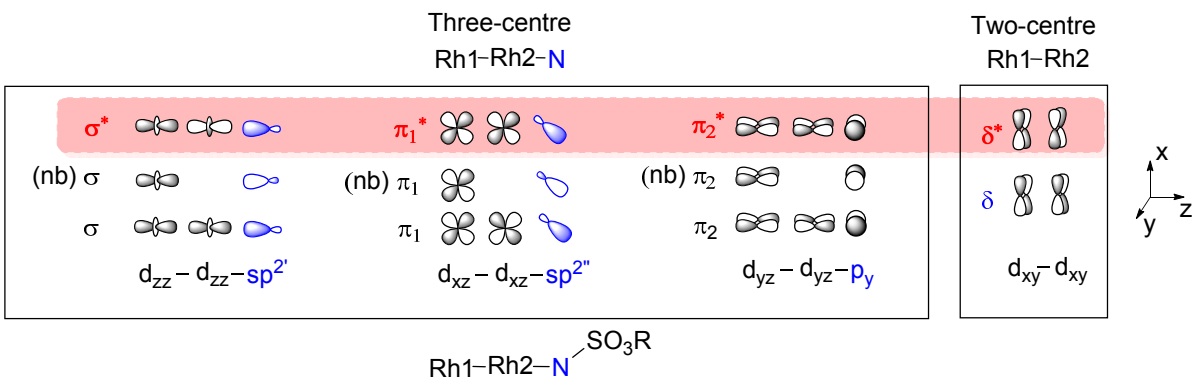

Fig. S2(a) The orbital bonding pattern of $Rh_2^{II,II}$-nitrene. Here, the σ-, π- and δ-symmetry orbitals are shown separately. The σ-, π- and δ-symmetry orbitals

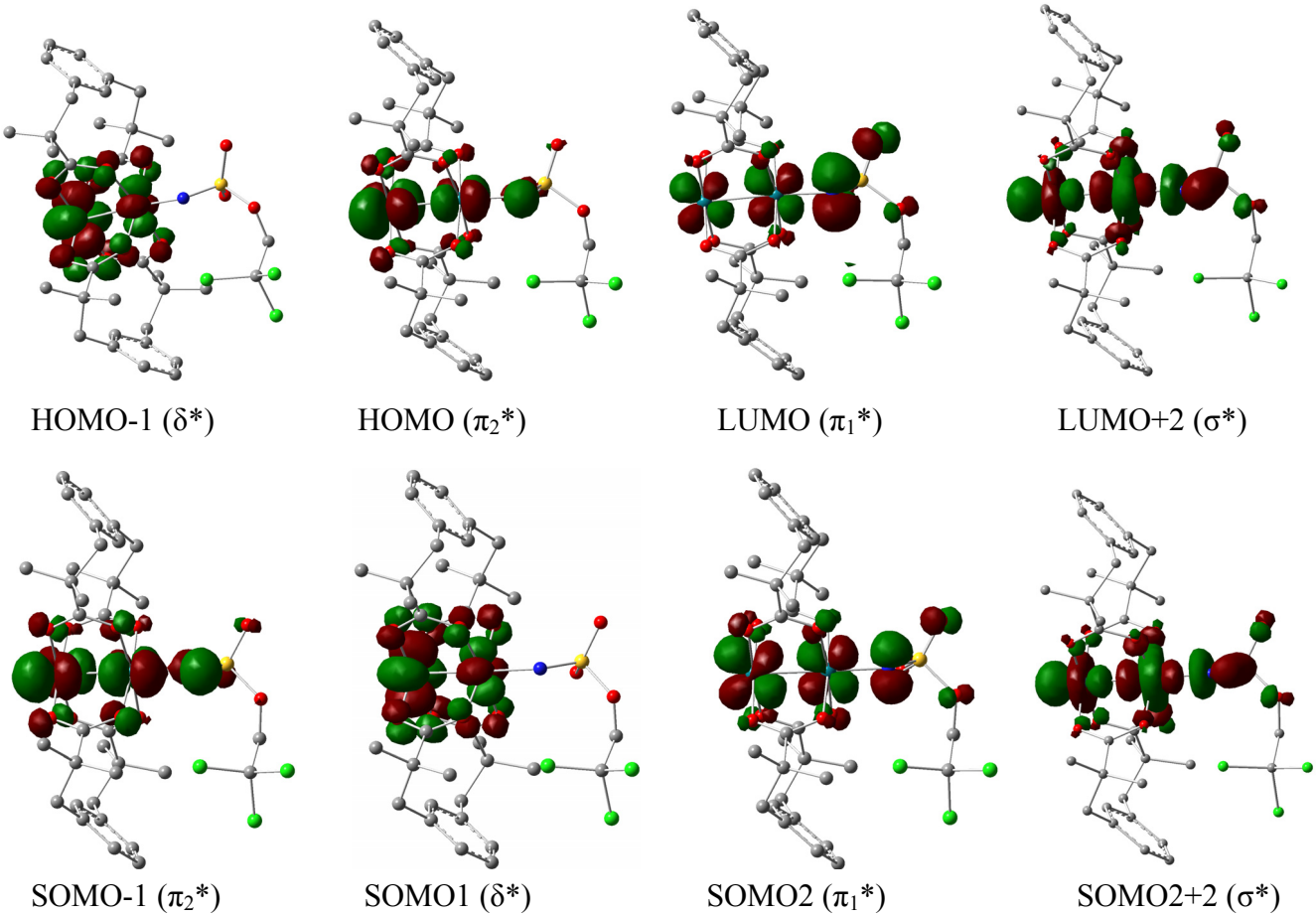

Fig. S2(b) Important Kohn-Sham frontier orbitals and electron configurations of **R-^{1}IM** and **R-^{3}IM**.

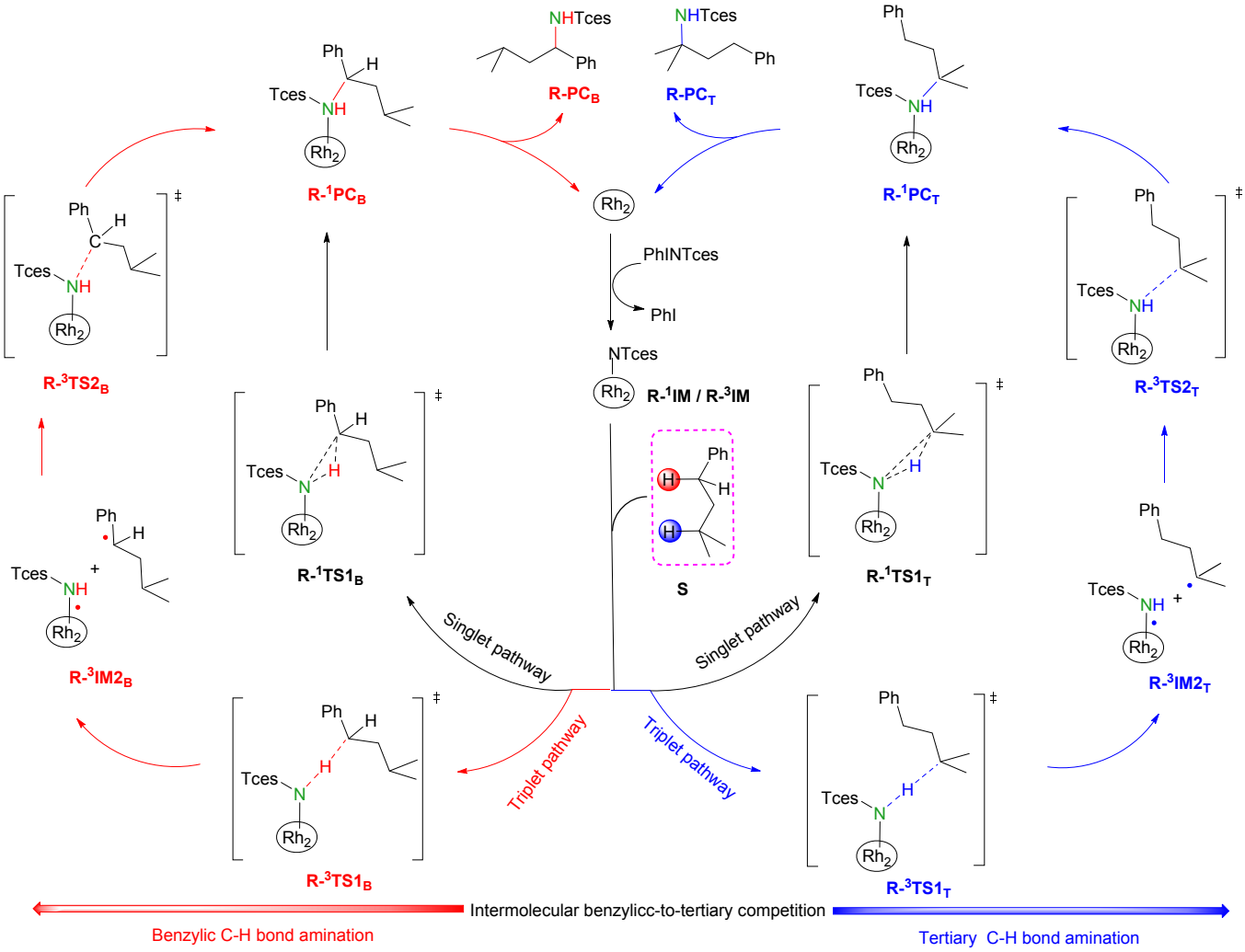

Fig. S3 Mechanisms of benzylic-to-tertiary competition for intramolecular C-H aminations. Herein, Rh$_2$=Rh$_2$(esp)$_2$

.

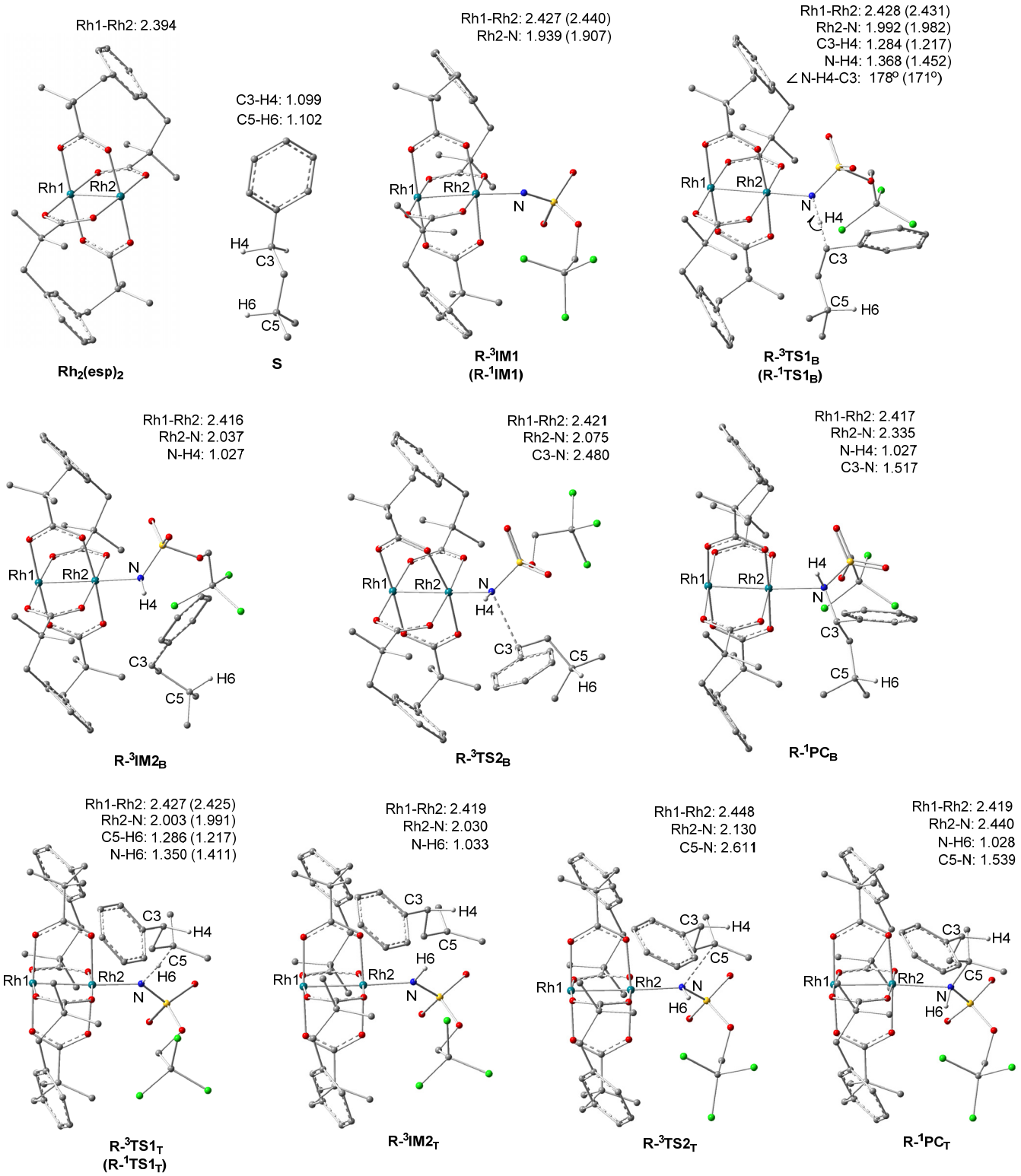

Fig. S4 Optimized structures and important geometrical parameters (bond lengths in Å, bond angles in degree) of the species for intermolecular C–H amination. Values without and with parentheses are for triplet and singlet states, respectively. For the sake of clarity, except for the reactive H4 and H6 atoms, the other H atoms are omitted.

.

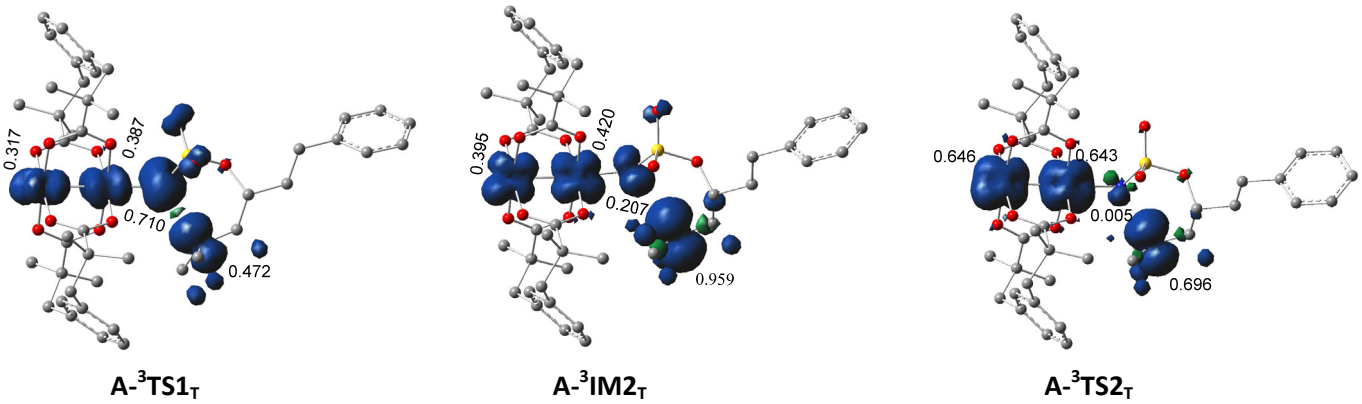

Fig. S5(a) Surface plots and values of the spin density distribution of triplet species for intramolecualr tertiary site C-H aminations.

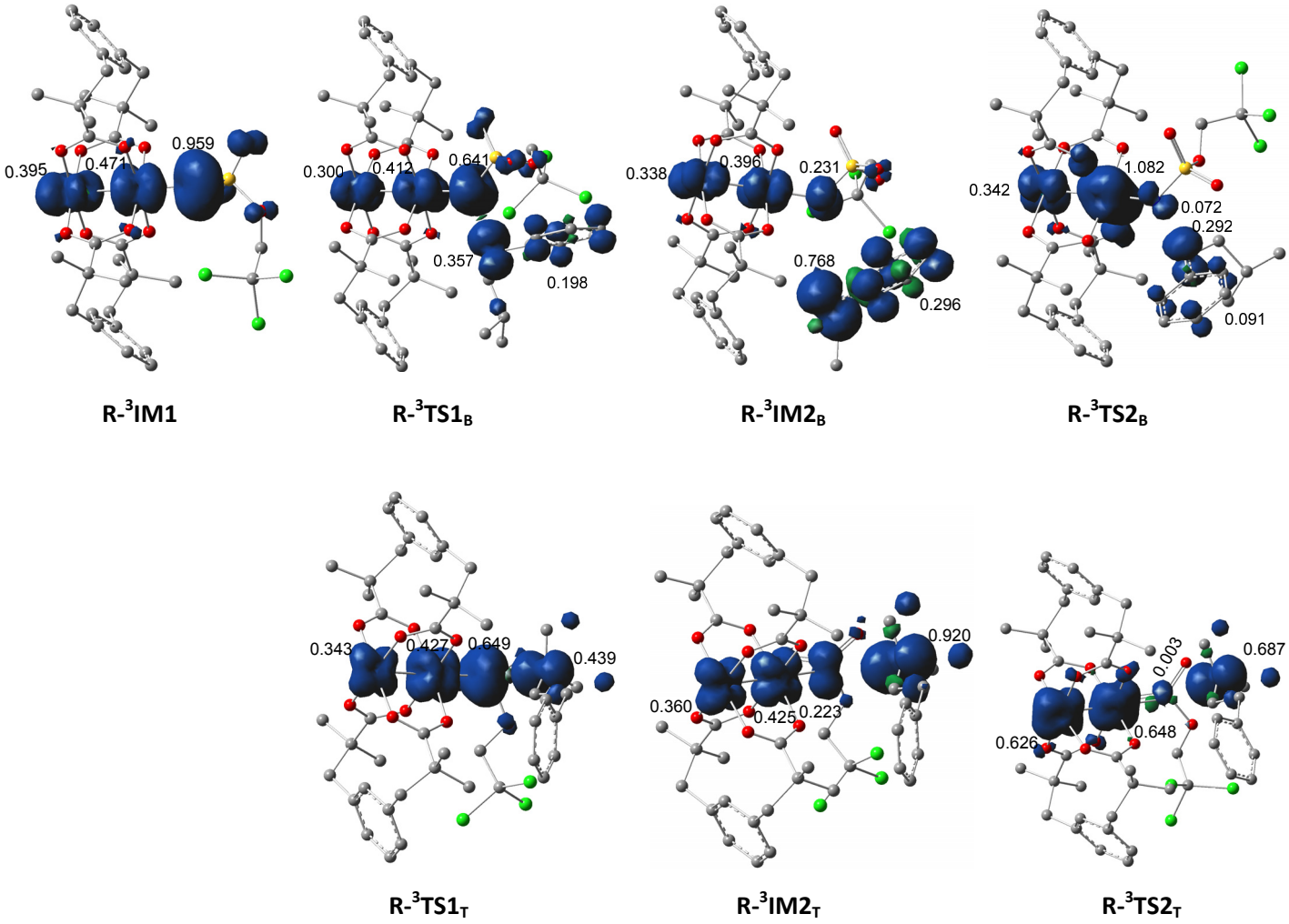

Fig. S5(b) Surface plots and values of the spin density distribution of triplet species for intermolecualr C-H aminations.

Table S1 Calculated NBO charge (in e) for selected atoms in inter- and intramolecular aminations.

Species	Rh1	Rh2	N	C3	H4	C5	H6	Ph group
$Rh_2(esp)_2$			—	—	—	—	—	—
R-^{1}IM1	0.835	1.101	-0.686	—	—	—	—	—
R-^{3}IM1	0.873	1.098	-0.691	—	—	—	—	—
S	—	—	—	-0.471	0.237	-0.242	0.232	-0.023
R-^{1}TS1$_B$	0.825	1.060	-0.870	-0.370	0.336	-0.233	0.238	0.136
R-^{3}TS1$_B$	0.845	1.081	-0.899	-0.368	0.357	-0.233	0.239	0.091
R-^{3}IM2$_B$	0.882	1.083	-1.056	-0.120	0.441	-0.229	0.237	-0.075
R-^{3}TS2$_B$	0.881	1.055	-1.102	0.034	0.436	-0.222	0.237	0.095
R-^{1}PC$_B$	0.840	0.912	-0.924	-0.066	0.468	-0.237	0.236	0.004
R-^{1}TS1$_T$	0.836	1.052	-0.858	-0.464	0.241	-0.106	0.323	-0.002
R-^{3}TS1$_T$	0.858	1.078	-0.913	-0.466	0.235	-0.097	0.349	-0.015
R-^{3}IM2$_T$	0.876	1.085	-1.074	-0.465	0.234	0.081	0.424	-0.024
R-^{3}TS2$_T$	0.895	1.057	-1.119	-0.460	0.240	0.211	0.423	-0.016
R-^{1}PC$_T$	0.854	0.906	-0.945	-0.467	0.242	0.168	0.441	-0.011
A-^{1}IM1	0.826	1.100	-0.690	-0.479	0.267	-0.240	0.232	-0.006
A-^{3}IM1	0.866	1.090	-0.686	-0.482	0.268	-0.240	0.232	-0.022
A-^{1}TS1$_B$	0.820	1.055	-0.838	-0.369	0.339	-0.240	0.232	0.101
A-^{3}TS1$_B$	0.846	1.080	-0.860	-0.385	0.352	-0.240	0.232	0.054
A-^{3}IM2$_B$	0.859	1.082	-1.036	-0.126	0.440	-0.245	0.231	-0.081
A-^{3}TS2$_B$	0.885	1.067	-1.096	-0.047	0.434	-0.244	0.232	-0.004
A-^{1}PC$_B$	0.828	0.911	-0.929	-0.072	0.464	-0.243	0.230	0.007
A-^{1}TS1$_T$	0.817	1.044	-0.842	-0.478	0.261	-0.077	0.327	-0.019
A-^{3}TS1$_T$	0.846	1.072	-0.868	-0.478	0.260	-0.106	0.345	-0.020
A-^{3}IM2$_T$	0.872	1.073	-1.057	-0.479	0.258	0.118	0.425	-0.023
A-^{3}TS2$_T$	0.900	1.056	-1.124	-0.478	0.243	0.201	0.418	-0.022
A-^{1}PC$_T$	0.846	0.905	-0.949	-0.477	0.262	0.158	0.456	-0.015

Table S2 Cartesian coordinates for the calculated structures.

A-^{3}IM1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.236997	-2.230357	0.800974
2	45	0	-0.389686	-0.241729	-0.307687
3	8	0	-2.579041	-2.486584	-0.745737
4	6	0	-2.609254	-1.616698	-1.703979
5	8	0	-1.813265	-0.587259	-1.775922
6	8	0	-2.623500	-1.125548	1.840119
7	6	0	-2.600267	0.158648	1.671104
8	8	0	-1.774668	0.763059	0.867908
9	8	0	1.038863	-0.092035	1.195721
10	6	0	0.978942	-0.894477	2.213946
11	8	0	0.114965	-1.857967	2.333089
12	8	0	0.158887	-3.295124	-0.272513
13	6	0	0.983068	-2.711977	-1.089356
14	8	0	0.956500	-1.435320	-1.337194
15	6	0	-3.602175	-1.786306	-2.840016
16	6	0	-4.397143	-0.450397	-2.998463
17	1	0	-3.684261	0.327554	-3.293328
18	1	0	-5.095451	-0.599042	-3.832432
19	6	0	-5.134951	-0.028798	-1.755441
20	6	0	-4.494785	0.773868	-0.799880
21	6	0	-6.448150	-0.455395	-1.507038
22	6	0	-5.122788	1.117907	0.406558
23	1	0	-3.495125	1.153497	-1.001136
24	6	0	-7.097069	-0.095606	-0.324161
25	1	0	-6.962635	-1.062163	-2.248827
26	6	0	-6.435532	0.677151	0.632467
27	1	0	-8.118724	-0.418187	-0.147377
28	1	0	-6.941084	0.952471	1.555310
29	6	0	-3.556531	1.043813	2.449156
30	6	0	-4.365444	1.915009	1.434491
31	1	0	-5.051400	2.527990	2.033501
32	1	0	-3.659725	2.589184	0.936014
33	6	0	1.994423	-3.588514	-1.807306
34	6	0	1.963743	-0.687032	3.352264
35	6	0	-4.540285	-2.962111	-2.565171
36	1	0	-5.257365	-3.053215	-3.388933
37	1	0	-3.982251	-3.898939	-2.485768
38	1	0	-5.094279	-2.823921	-1.633259
39	6	0	-2.801857	-2.033998	-4.134215
40	1	0	-2.233834	-2.968521	-4.069901
41	1	0	-3.495056	-2.117414	-4.978081

42	1	0	-2.107324	-1.212146	-4.329026
43	6	0	-2.710287	1.988516	3.325648
44	1	0	-3.374793	2.676646	3.858990
45	1	0	-2.138391	1.424212	4.070534
46	1	0	-2.014084	2.568401	2.713019
47	6	0	-4.485802	0.193735	3.316504
48	1	0	-3.916831	-0.403605	4.034298
49	1	0	-5.162359	0.852972	3.871973
50	1	0	-5.083924	-0.493081	2.711967
51	6	0	2.681829	-4.516553	-0.755988
52	1	0	1.902671	-5.141618	-0.305668
53	1	0	3.354711	-5.176903	-1.317962
54	6	0	1.207694	-4.475376	-2.795772
55	1	0	0.450098	-5.068441	-2.275243
56	1	0	0.715710	-3.864574	-3.559972
57	1	0	1.901066	-5.156065	-3.300970
58	6	0	2.683507	-2.043281	3.633586
59	1	0	3.357254	-1.872928	4.483035
60	1	0	1.921996	-2.764045	3.952814
61	6	0	1.146060	-0.290284	4.597728
62	1	0	0.634474	0.664570	4.435272
63	1	0	0.400603	-1.053787	4.837597
64	1	0	1.820511	-0.172631	5.452657
65	6	0	2.970956	0.414915	3.017112
66	1	0	3.647001	0.556822	3.868241
67	1	0	3.572016	0.162623	2.138611
68	1	0	2.460207	1.360677	2.814949
69	6	0	3.021811	-2.744082	-2.559875
70	1	0	3.586970	-2.095924	-1.885215
71	1	0	3.726716	-3.406296	-3.075594
72	1	0	2.538808	-2.103910	-3.302272
73	6	0	3.445094	-3.786396	0.318632
74	6	0	2.783651	-3.327416	1.467470
75	6	0	4.818166	-3.529781	0.190480
76	6	0	3.449231	-2.585413	2.455135
77	1	0	1.730381	-3.559332	1.598839
78	6	0	5.501691	-2.817529	1.178688
79	1	0	5.350618	-3.893706	-0.686087
80	6	0	4.820539	-2.335386	2.297269
81	1	0	6.565568	-2.628144	1.070752
82	1	0	5.352734	-1.769358	3.057914
83	8	0	0.178197	2.985631	1.114766
84	16	0	-0.268629	2.935118	-0.275171
85	8	0	-1.640139	3.277650	-0.621342
86	7	0	0.124384	1.508230	-0.987337

87	6	0	1.856735	4.557406	-0.583855
88	6	0	3.086424	3.832399	-1.095504
89	6	0	3.196783	2.375269	-0.683079
90	1	0	3.118770	3.923223	-2.191983
91	1	0	3.956697	4.390222	-0.717718
92	1	0	3.112756	2.296117	0.413217
93	1	0	2.325806	1.815040	-1.060880
94	6	0	4.448361	1.677890	-1.149550
95	6	0	4.613801	0.308215	-0.898230
96	6	0	5.462194	2.342229	-1.847435
97	6	0	5.748720	-0.365410	-1.336365
98	1	0	3.831423	-0.235284	-0.359988
99	6	0	6.603458	1.670176	-2.280158
100	1	0	5.364858	3.404327	-2.065479
101	6	0	6.751022	0.311636	-2.028719
102	1	0	5.847233	-1.431315	-1.138947
103	1	0	7.376773	2.214760	-2.820122
104	1	0	7.637912	-0.219849	-2.370119
105	8	0	0.651466	3.945403	-1.156414
106	1	0	1.785554	4.463810	0.508771
107	6	0	1.814882	6.018934	-1.011184
108	6	0	1.044599	6.966279	-0.089892
109	1	0	1.393142	6.059111	-2.027117
110	1	0	2.850123	6.380311	-1.101348
111	1	0	1.583999	6.996795	0.872626
112	6	0	1.052279	8.370672	-0.678920
113	1	0	0.572065	9.090395	-0.005198
114	1	0	2.071644	8.725933	-0.877544
115	1	0	0.503248	8.394534	-1.630344
116	6	0	-0.378813	6.501535	0.190022
117	1	0	-0.939148	6.338445	-0.739832
118	1	0	-0.403483	5.563442	0.756299
119	1	0	-0.919762	7.251481	0.780529

A-^{1}IM1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.193511	-2.253592	0.746273
2	45	0	-0.372442	-0.179395	-0.253150
3	8	0	-2.523356	-2.505747	-0.793576
4	6	0	-2.538526	-1.621073	-1.739398
5	8	0	-1.757180	-0.581605	-1.774206
6	8	0	-2.601610	-1.194329	1.821934

7	6	0	-2.612622	0.091302	1.689954
8	8	0	-1.804252	0.748037	0.907475
9	8	0	0.987884	-0.041394	1.277340
10	6	0	0.969560	-0.910328	2.244607
11	8	0	0.147634	-1.911190	2.288784
12	8	0	0.232625	-3.242938	-0.364048
13	6	0	1.067928	-2.600932	-1.122584
14	8	0	1.054912	-1.311654	-1.288576
15	6	0	-3.506421	-1.782302	-2.898874
16	6	0	-4.346370	-0.469007	-3.015795
17	1	0	-3.658515	0.342629	-3.277870
18	1	0	-5.033927	-0.612168	-3.859749
19	6	0	-5.105638	-0.115942	-1.764205
20	6	0	-4.506245	0.691061	-0.786330
21	6	0	-6.396752	-0.611974	-1.529520
22	6	0	-5.151552	0.975372	0.426759
23	1	0	-3.524067	1.119121	-0.974834
24	6	0	-7.062059	-0.316752	-0.337985
25	1	0	-6.881930	-1.222401	-2.287783
26	6	0	-6.440536	0.463630	0.639339
27	1	0	-8.066062	-0.695052	-0.170850
28	1	0	-6.960126	0.689494	1.567825
29	6	0	-3.595942	0.934349	2.481459
30	6	0	-4.434061	1.786169	1.473287
31	1	0	-5.147481	2.364244	2.075119
32	1	0	-3.750600	2.493190	0.989065
33	6	0	2.096113	-3.434707	-1.871766
34	6	0	1.947191	-0.732097	3.390822
35	6	0	-4.406352	-2.999336	-2.683163
36	1	0	-5.095254	-3.093504	-3.530403
37	1	0	-3.815451	-3.916459	-2.612183
38	1	0	-4.991504	-2.907654	-1.764709
39	6	0	-2.680583	-1.949119	-4.189193
40	1	0	-2.085383	-2.868194	-4.156700
41	1	0	-3.358114	-2.015350	-5.047193
42	1	0	-2.008429	-1.099179	-4.335792
43	6	0	-2.782992	1.900437	3.366096
44	1	0	-3.470568	2.556413	3.910757
45	1	0	-2.186606	1.349568	4.102002
46	1	0	-2.111123	2.514352	2.758906
47	6	0	-4.494574	0.043793	3.339863
48	1	0	-3.904410	-0.542832	4.049523
49	1	0	-5.192389	0.672656	3.904307
50	1	0	-5.069192	-0.656092	2.727660
51	6	0	2.785692	-4.399347	-0.854415

52	1	0	2.009440	-5.055196	-0.444487
53	1	0	3.476937	-5.023584	-1.435254
54	6	0	1.326638	-4.286020	-2.903132
55	1	0	0.569581	-4.905570	-2.413896
56	1	0	0.835514	-3.646884	-3.644452
57	1	0	2.029718	-4.938707	-3.431560
58	6	0	2.683383	-2.088216	3.625228
59	1	0	3.344034	-1.942080	4.489371
60	1	0	1.928293	-2.830755	3.907592
61	6	0	1.118073	-0.394864	4.647357
62	1	0	0.587897	0.554734	4.517214
63	1	0	0.387629	-1.181014	4.859123
64	1	0	1.788301	-0.294469	5.507701
65	6	0	2.936677	0.398292	3.100381
66	1	0	3.609214	0.518952	3.957302
67	1	0	3.543329	0.190170	2.213997
68	1	0	2.409779	1.342273	2.933458
69	6	0	3.120003	-2.549554	-2.579942
70	1	0	3.686111	-1.938806	-1.872738
71	1	0	3.824180	-3.180566	-3.134403
72	1	0	2.633282	-1.868645	-3.282803
73	6	0	3.523216	-3.708318	0.263807
74	6	0	2.832949	-3.286021	1.410271
75	6	0	4.900554	-3.455423	0.182693
76	6	0	3.473583	-2.579825	2.439928
77	1	0	1.777812	-3.524064	1.506763
78	6	0	5.559472	-2.779492	1.212714
79	1	0	5.455466	-3.793741	-0.690095
80	6	0	4.849508	-2.329357	2.326845
81	1	0	6.627426	-2.594886	1.141843
82	1	0	5.362862	-1.792107	3.120546
83	8	0	0.140879	2.907977	1.098803
84	16	0	-0.317920	2.869941	-0.287864
85	8	0	-1.706341	3.188001	-0.609784
86	7	0	0.021017	1.477902	-1.122265
87	6	0	1.742549	4.573489	-0.552434
88	6	0	2.989854	3.880183	-1.062335
89	6	0	3.100604	2.411170	-0.696365
90	1	0	3.039219	4.006285	-2.154380
91	1	0	3.850396	4.428656	-0.650145
92	1	0	2.977152	2.288817	0.391721
93	1	0	2.246447	1.857612	-1.132655
94	6	0	4.375955	1.746405	-1.141692
95	6	0	4.606370	0.398619	-0.830343
96	6	0	5.355915	2.426398	-1.873869

97	6	0	5.770972	-0.238651	-1.243849
98	1	0	3.851929	-0.158388	-0.266562
99	6	0	6.526013	1.790974	-2.281744
100	1	0	5.209835	3.472868	-2.134399
101	6	0	6.737777	0.453142	-1.970687
102	1	0	5.921368	-1.288066	-0.999275
103	1	0	7.272008	2.347477	-2.847285
104	1	0	7.648026	-0.050722	-2.291794
105	8	0	0.567485	3.932736	-1.147073
106	1	0	1.663419	4.465816	0.538257
107	6	0	1.670022	6.038898	-0.960231
108	6	0	0.872621	6.950383	-0.025865
109	1	0	1.252398	6.085413	-1.977547
110	1	0	2.697522	6.424683	-1.039026
111	1	0	1.406439	6.975516	0.939950
112	6	0	0.847307	8.365699	-0.587054
113	1	0	0.343448	9.058932	0.097137
114	1	0	1.858256	8.751716	-0.770520
115	1	0	0.304596	8.394329	-1.541933
116	6	0	-0.539397	6.442994	0.237281
117	1	0	-1.091189	6.287048	-0.698929
118	1	0	-0.542097	5.491610	0.781821
119	1	0	-1.102073	7.164854	0.842280

A-^{3}TS1$_B$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.267073	-2.577058	0.143995
2	45	0	-0.096485	-0.187270	-0.098584
3	8	0	-1.036542	-2.916930	-1.407958
4	6	0	-1.580397	-1.906074	-2.005237
5	8	0	-1.370649	-0.665820	-1.667318
6	8	0	-1.277471	-2.666225	1.499125
7	6	0	-1.898289	-1.573485	1.809821
8	8	0	-1.622086	-0.411014	1.291773
9	8	0	1.296257	0.078616	1.472733
10	6	0	1.825021	-0.962892	2.040186
11	8	0	1.555465	-2.187347	1.704859
12	8	0	1.819103	-2.396015	-1.215390
13	6	0	2.147675	-1.231353	-1.687786
14	8	0	1.506093	-0.134567	-1.419143
15	6	0	-2.517697	-2.150746	-3.175951

16	6	0	-3.917344	-1.559157	-2.810285
17	1	0	-3.809721	-0.470101	-2.742488
18	1	0	-4.580288	-1.779998	-3.657259
19	6	0	-4.493722	-2.087527	-1.524210
20	6	0	-4.220362	-1.410749	-0.328412
21	6	0	-5.280646	-3.248028	-1.478713
22	6	0	-4.696965	-1.876186	0.904635
23	1	0	-3.644578	-0.489632	-0.359839
24	6	0	-5.772839	-3.717580	-0.258521
25	1	0	-5.517641	-3.773772	-2.401053
26	6	0	-5.481098	-3.039641	0.927843
27	1	0	-6.391189	-4.609796	-0.232977
28	1	0	-5.873844	-3.405127	1.873922
29	6	0	-3.013388	-1.617212	2.840327
30	6	0	-4.331509	-1.125537	2.157652
31	1	0	-5.123623	-1.213400	2.912865
32	1	0	-4.207798	-0.060985	1.925211
33	6	0	3.329958	-1.164418	-2.642419
34	6	0	2.787365	-0.784984	3.207567
35	6	0	-2.616551	-3.646482	-3.478045
36	1	0	-3.290293	-3.799248	-4.328950
37	1	0	-1.636681	-4.061109	-3.731085
38	1	0	-3.001241	-4.203622	-2.620307
39	6	0	-1.974693	-1.389643	-4.399040
40	1	0	-1.005814	-1.792606	-4.713480
41	1	0	-2.673676	-1.499437	-5.235266
42	1	0	-1.855847	-0.326402	-4.174267
43	6	0	-2.658160	-0.634722	3.971898
44	1	0	-3.477317	-0.607253	4.698483
45	1	0	-1.750754	-0.954273	4.496882
46	1	0	-2.499090	0.372499	3.576739
47	6	0	-3.179477	-3.035236	3.387878
48	1	0	-2.255868	-3.386661	3.856342
49	1	0	-3.976259	-3.040317	4.140356
50	1	0	-3.439867	-3.741900	2.595557
51	6	0	4.517510	-1.979890	-2.043484
52	1	0	4.183630	-3.017955	-1.932288
53	1	0	5.315692	-1.967224	-2.797022
54	6	0	2.892017	-1.839932	-3.958480
55	1	0	2.576781	-2.872940	-3.783749
56	1	0	2.064350	-1.291181	-4.420020
57	1	0	3.731310	-1.842107	-4.662464
58	6	0	4.052417	-1.667202	2.960172
59	1	0	4.692964	-1.552631	3.844386
60	1	0	3.725355	-2.712171	2.921023

61	6	0	2.059560	-1.308281	4.463904
62	1	0	1.168109	-0.707689	4.675428
63	1	0	1.756710	-2.350943	4.332102
64	1	0	2.728342	-1.240644	5.328753
65	6	0	3.182244	0.676909	3.403140
66	1	0	3.790614	0.771544	4.309757
67	1	0	3.774695	1.041232	2.558949
68	1	0	2.300496	1.315446	3.507136
69	6	0	3.735072	0.286985	-2.901400
70	1	0	4.024872	0.793219	-1.977019
71	1	0	4.584955	0.312152	-3.594042
72	1	0	2.909693	0.855066	-3.338968
73	6	0	5.041214	-1.465331	-0.727058
74	6	0	4.396073	-1.813702	0.468387
75	6	0	6.170783	-0.635266	-0.660964
76	6	0	4.821503	-1.319820	1.710612
77	1	0	3.554363	-2.497767	0.433205
78	6	0	6.635895	-0.171092	0.571672
79	1	0	6.690828	-0.365541	-1.577725
80	6	0	5.958838	-0.498425	1.750046
81	1	0	7.523502	0.454076	0.614003
82	1	0	6.316885	-0.125260	2.707089
83	8	0	-1.954407	2.733123	1.683613
84	16	0	-1.985240	2.398951	0.261136
85	8	0	-3.096058	1.655533	-0.299339
86	7	0	-0.542062	1.760400	-0.214522
87	6	0	-1.331843	4.978956	-0.045336
88	6	0	0.114611	4.986906	-0.519358
89	6	0	0.944052	3.891885	0.095220
90	1	0	0.121028	4.923337	-1.617339
91	1	0	0.554350	5.965780	-0.264632
92	1	0	0.842461	3.850789	1.189449
93	1	0	0.316681	2.773576	-0.145564
94	6	0	2.313337	3.653497	-0.346246
95	6	0	3.120144	2.804245	0.434655
96	6	0	2.868122	4.211495	-1.512476
97	6	0	4.437812	2.553917	0.094203
98	1	0	2.675547	2.341954	1.314147
99	6	0	4.192903	3.963290	-1.851246
100	1	0	2.264911	4.863307	-2.142574
101	6	0	4.985084	3.141394	-1.049211
102	1	0	5.042284	1.892328	0.712923
103	1	0	4.613550	4.417454	-2.747152
104	1	0	6.021711	2.945241	-1.321527
105	8	0	-1.996976	3.801707	-0.586971

106	1	0	-1.368806	4.909493	1.052978
107	6	0	-2.145623	6.170775	-0.524746
108	6	0	-3.343643	6.532184	0.355711
109	1	0	-2.481003	5.963416	-1.552530
110	1	0	-1.479429	7.043889	-0.591554
111	1	0	-2.942813	6.843193	1.336025
112	6	0	-4.086335	7.718283	-0.245340
113	1	0	-4.909420	8.044447	0.401701
114	1	0	-3.423832	8.578998	-0.403941
115	1	0	-4.520739	7.452328	-1.218922
116	6	0	-4.289510	5.360470	0.592211
117	1	0	-4.648371	4.940346	-0.356667
118	1	0	-3.810673	4.546757	1.148295
119	1	0	-5.164927	5.684515	1.168415

A-^{1}TS1$_{B}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.166807	-2.571484	0.239793
2	45	0	-0.116977	-0.174119	-0.103144
3	8	0	-1.125304	-2.995137	-1.287357
4	6	0	-1.635506	-1.999094	-1.938698
5	8	0	-1.383279	-0.751068	-1.673515
6	8	0	-1.402394	-2.540864	1.580273
7	6	0	-1.991639	-1.415049	1.822933
8	8	0	-1.667117	-0.283099	1.265431
9	8	0	1.227267	0.134411	1.472811
10	6	0	1.743261	-0.893869	2.083057
11	8	0	1.452736	-2.119072	1.784077
12	8	0	1.730289	-2.487426	-1.123479
13	6	0	2.108030	-1.353092	-1.629415
14	8	0	1.518826	-0.217683	-1.403584
15	6	0	-2.576834	-2.280949	-3.098775
16	6	0	-3.933203	-1.558254	-2.822880
17	1	0	-3.742011	-0.478458	-2.827918
18	1	0	-4.587970	-1.787861	-3.673912
19	6	0	-4.586824	-1.948097	-1.523297
20	6	0	-4.272648	-1.231359	-0.360818
21	6	0	-5.483413	-3.023079	-1.431231
22	6	0	-4.813100	-1.577726	0.885023
23	1	0	-3.617383	-0.368110	-0.429810
24	6	0	-6.043880	-3.369391	-0.199230
25	1	0	-5.749929	-3.579157	-2.327295
26	6	0	-5.708049	-2.655843	0.954158

27	1	0	-6.747102	-4.194774	-0.138447
28	1	0	-6.149551	-2.926991	1.910748
29	6	0	-3.132327	-1.370258	2.826409
30	6	0	-4.397728	-0.801274	2.106413
31	1	0	-5.202162	-0.790622	2.853643
32	1	0	-4.181982	0.237089	1.827544
33	6	0	3.299172	-1.381062	-2.578372
34	6	0	2.703789	-0.689002	3.245984
35	6	0	-2.782698	-3.786963	-3.266799
36	1	0	-3.464263	-3.966693	-4.106300
37	1	0	-1.834807	-4.291505	-3.473054
38	1	0	-3.208907	-4.235116	-2.365712
39	6	0	-1.954815	-1.679709	-4.373311
40	1	0	-1.012742	-2.180873	-4.621247
41	1	0	-2.642699	-1.817382	-5.214690
42	1	0	-1.761365	-0.611236	-4.244817
43	6	0	-2.736959	-0.395277	3.951539
44	1	0	-3.564137	-0.308399	4.664437
45	1	0	-1.858236	-0.761099	4.495139
46	1	0	-2.511674	0.594685	3.545203
47	6	0	-3.403697	-2.764270	3.392368
48	1	0	-2.521581	-3.158549	3.904670
49	1	0	-4.228806	-2.708456	4.111844
50	1	0	-3.672972	-3.470704	2.602875
51	6	0	4.451622	-2.207517	-1.928089
52	1	0	4.079272	-3.226568	-1.771804
53	1	0	5.256855	-2.260361	-2.672303
54	6	0	2.841373	-2.111955	-3.857614
55	1	0	2.478170	-3.117438	-3.625555
56	1	0	2.041320	-1.555071	-4.356690
57	1	0	3.683991	-2.192356	-4.553083
58	6	0	3.942043	-1.622397	3.051726
59	1	0	4.578802	-1.484407	3.935312
60	1	0	3.580944	-2.656957	3.063695
61	6	0	1.948845	-1.131334	4.518189
62	1	0	1.079054	-0.489408	4.695383
63	1	0	1.608150	-2.166854	4.429466
64	1	0	2.614367	-1.050723	5.384343
65	6	0	3.146737	0.766160	3.385342
66	1	0	3.709440	0.884515	4.318200
67	1	0	3.802223	1.063768	2.561769
68	1	0	2.289455	1.445014	3.408486
69	6	0	3.765873	0.033889	-2.918059
70	1	0	4.102288	0.566427	-2.025299
71	1	0	4.599454	-0.017174	-3.628695

72	1	0	2.958070	0.619619	-3.365177
73	6	0	4.986941	-1.656371	-0.630159
74	6	0	4.296024	-1.889341	0.567993
75	6	0	6.182383	-0.922552	-0.580183
76	6	0	4.741078	-1.374733	1.795427
77	1	0	3.408590	-2.512328	0.548322
78	6	0	6.665302	-0.439954	0.639112
79	1	0	6.739938	-0.745384	-1.497488
80	6	0	5.943065	-0.649205	1.818215
81	1	0	7.603200	0.107765	0.670580
82	1	0	6.317642	-0.263369	2.763766
83	8	0	-1.606900	2.724526	1.539823
84	16	0	-1.845427	2.437813	0.127576
85	8	0	-3.062008	1.777164	-0.310422
86	7	0	-0.575819	1.693151	-0.654225
87	6	0	-1.100522	4.980200	-0.145263
88	6	0	0.322032	4.849400	-0.663883
89	6	0	1.046937	3.638396	-0.132174
90	1	0	0.300600	4.845588	-1.763513
91	1	0	0.884161	5.749726	-0.366724
92	1	0	0.896440	3.501419	0.948367
93	1	0	0.411838	2.640678	-0.531201
94	6	0	2.436281	3.398945	-0.529817
95	6	0	3.181142	2.466114	0.212067
96	6	0	3.066312	4.070027	-1.591775
97	6	0	4.523389	2.256407	-0.049065
98	1	0	2.670555	1.901081	0.989328
99	6	0	4.412154	3.850903	-1.860441
100	1	0	2.508178	4.788755	-2.189897
101	6	0	5.146998	2.952508	-1.086070
102	1	0	5.082871	1.533883	0.542017
103	1	0	4.894348	4.389671	-2.674098
104	1	0	6.201007	2.778802	-1.301057
105	8	0	-1.891247	3.878619	-0.660566
106	1	0	-1.105166	4.916029	0.953866
107	6	0	-1.808042	6.245884	-0.601947
108	6	0	-2.957964	6.704424	0.298202
109	1	0	-2.174495	6.080233	-1.626817
110	1	0	-1.065870	7.055664	-0.670514
111	1	0	-2.518032	6.977309	1.273029
112	6	0	-3.605841	7.951034	-0.289839
113	1	0	-4.388037	8.343988	0.370406
114	1	0	-2.874390	8.752342	-0.456383
115	1	0	-4.075611	7.726513	-1.257415
116	6	0	-3.995237	5.615438	0.545764

117	1	0	-4.396669	5.225067	-0.398435
118	1	0	-3.579230	4.764665	1.096810
119	1	0	-4.834316	6.011683	1.131001

A-^{3}IM2$_B$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.847201	1.425966	1.304747
2	45	0	-0.453383	0.232142	-0.274499
3	8	0	-2.410444	-0.413158	2.075774
4	6	0	-1.892028	-1.499997	1.595961
5	8	0	-1.057174	-1.532873	0.597736
6	8	0	-3.385766	1.376932	-0.039426
7	6	0	-3.204178	0.817934	-1.195100
8	8	0	-2.078895	0.276589	-1.559103
9	8	0	0.159407	2.049201	-1.041757
10	6	0	-0.332522	3.149369	-0.557037
11	8	0	-1.183339	3.198845	0.422344
12	8	0	-0.288410	1.430934	2.648079
13	6	0	0.829216	0.852417	2.333460
14	8	0	1.051443	0.312584	1.172726
15	6	0	-2.251003	-2.842927	2.205737
16	6	0	-2.938006	-3.703513	1.094892
17	1	0	-2.175982	-3.934677	0.341050
18	1	0	-3.239038	-4.646193	1.570525
19	6	0	-4.113416	-3.034820	0.433669
20	6	0	-3.899824	-2.255777	-0.712559
21	6	0	-5.416242	-3.145011	0.941833
22	6	0	-4.950641	-1.572448	-1.340111
23	1	0	-2.899897	-2.195353	-1.136714
24	6	0	-6.476015	-2.484425	0.315724
25	1	0	-5.600586	-3.761385	1.818979
26	6	0	-6.246053	-1.698066	-0.815701
27	1	0	-7.483537	-2.586690	0.707654
28	1	0	-7.075022	-1.190536	-1.303571
29	6	0	-4.345509	0.785202	-2.194637
30	6	0	-4.651677	-0.709326	-2.537562
31	1	0	-5.499788	-0.699768	-3.234843
32	1	0	-3.783463	-1.112522	-3.071911
33	6	0	1.926510	0.824471	3.384601
34	6	0	0.128627	4.462262	-1.170894
35	6	0	2.334885	2.303626	3.687561
36	1	0	1.493440	2.779159	4.204531
37	1	0	3.175407	2.258683	4.392032

38	6	0	0.848806	5.289293	-0.057601
39	1	0	1.217105	6.205685	-0.536797
40	1	0	0.091177	5.581713	0.678479
41	6	0	2.697662	3.106598	2.467002
42	6	0	1.700101	3.833338	1.801679
43	6	0	4.001827	3.127754	1.950368
44	6	0	1.969634	4.559682	0.633656
45	1	0	0.689789	3.837398	2.205733
46	6	0	4.290049	3.854765	0.792709
47	1	0	4.792253	2.584327	2.462223
48	6	0	3.281738	4.563884	0.135438
49	1	0	5.303252	3.868542	0.402121
50	1	0	3.513811	5.137561	-0.759200
51	8	0	1.261688	-2.208888	-3.579123
52	16	0	0.458669	-2.155980	-2.363221
53	8	0	-0.946054	-2.502687	-2.346903
54	7	0	0.662297	-0.684262	-1.682176
55	8	0	1.095993	-3.217720	-1.281629
56	6	0	3.307873	-1.402264	-0.385960
57	1	0	1.424941	-0.167005	-2.124960
58	1	0	2.732480	-0.860063	0.360559
59	6	0	3.898100	-0.593820	-1.388191
60	6	0	4.592354	-1.081442	-2.529283
61	6	0	3.761379	0.822080	-1.274386
62	6	0	5.125521	-0.215338	-3.469153
63	1	0	4.693140	-2.154036	-2.680518
64	6	0	4.304986	1.677020	-2.216679
65	1	0	3.214031	1.226959	-0.419189
66	6	0	4.995325	1.168560	-3.321930
67	1	0	5.645650	-0.621176	-4.335535
68	1	0	4.193007	2.753754	-2.088604
69	1	0	5.419547	1.842253	-4.063955
70	6	0	3.297391	-2.896043	-0.271811
71	1	0	2.754961	-3.125058	0.658824
72	6	0	4.707708	-3.498346	-0.136961
73	6	0	4.783220	-5.011395	0.091526
74	1	0	5.315728	-3.240957	-1.016009
75	1	0	4.429918	-5.523071	-0.819106
76	6	0	-3.878265	1.489887	-3.481918
77	1	0	-4.668739	1.428326	-4.237380
78	1	0	-3.670293	2.549169	-3.295716
79	1	0	-2.974357	1.019025	-3.877524
80	6	0	-5.578914	1.482644	-1.619997
81	1	0	-5.365181	2.529312	-1.386444
82	1	0	-6.389276	1.448604	-2.356888

83	1	0	-5.918469	0.999438	-0.700620
84	6	0	-0.942077	-3.545656	2.613881
85	1	0	-0.418849	-2.983089	3.395230
86	1	0	-1.169441	-4.541919	3.008369
87	1	0	-0.277544	-3.646814	1.750266
88	6	0	-3.170315	-2.658291	3.412393
89	1	0	-3.408804	-3.638074	3.841564
90	1	0	-2.688725	-2.048704	4.182808
91	1	0	-4.102157	-2.161254	3.130966
92	6	0	-1.111277	5.248692	-1.632616
93	1	0	-0.800317	6.222653	-2.025772
94	1	0	-1.638635	4.715554	-2.430548
95	1	0	-1.805329	5.407504	-0.802979
96	6	0	1.066743	4.205485	-2.351581
97	1	0	0.560898	3.640136	-3.139033
98	1	0	1.398224	5.163292	-2.768695
99	1	0	1.943900	3.628412	-2.047373
100	6	0	3.133217	0.016553	2.906239
101	1	0	3.895939	0.004096	3.693013
102	1	0	2.851311	-1.018353	2.684289
103	1	0	3.576187	0.441815	2.000801
104	6	0	1.349301	0.207256	4.671272
105	1	0	1.078890	-0.842388	4.515827
106	1	0	2.102841	0.248794	5.464954
107	1	0	0.458886	0.749923	4.998163
108	6	0	2.488599	-3.570412	-1.379722
109	1	0	2.499351	-4.661006	-1.261301
110	1	0	2.858603	-3.336750	-2.385337
111	1	0	5.197990	-2.992276	0.710605
112	6	0	6.234247	-5.420760	0.310977
113	1	0	6.635393	-4.959135	1.224067
114	1	0	6.334780	-6.507402	0.419663
115	1	0	6.873505	-5.107239	-0.523630
116	6	0	3.913133	-5.465395	1.256938
117	1	0	4.047891	-6.534990	1.457783
118	1	0	4.177989	-4.921367	2.174947
119	1	0	2.843963	-5.300060	1.073264

A-^{3}TS2$_B$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.627720	-1.375378	1.504688
2	45	0	0.458211	-0.223601	-0.299516
3	8	0	2.420341	0.462609	2.055004

4	6	0	2.117341	1.517239	1.362442
5	8	0	1.360514	1.518170	0.305735
6	8	0	3.208043	-1.694150	0.236461
7	6	0	3.128689	-1.371522	-1.018586
8	8	0	2.072761	-0.824298	-1.532938
9	8	0	-0.481311	-2.002185	-0.806329
10	6	0	-0.121992	-3.088713	-0.191647
11	8	0	0.726590	-3.133791	0.789823
12	8	0	0.060779	-1.019871	2.797668
13	6	0	-0.928862	-0.264225	2.418150
14	8	0	-1.030086	0.222632	1.228712
15	6	0	2.657911	2.872286	1.782064
16	6	0	3.449329	3.463735	0.569487
17	1	0	2.724213	3.671930	-0.226572
18	1	0	3.869794	4.421436	0.903517
19	6	0	4.529904	2.558321	0.040564
20	6	0	4.223744	1.639956	-0.974906
21	6	0	5.835712	2.586936	0.552701
22	6	0	5.182977	0.741014	-1.461838
23	1	0	3.224794	1.636331	-1.406387
24	6	0	6.807215	1.711679	0.061271
25	1	0	6.092080	3.306544	1.327121
26	6	0	6.483277	0.790358	-0.936473
27	1	0	7.819161	1.751875	0.453363
28	1	0	7.242433	0.112115	-1.319441
29	6	0	4.309049	-1.639633	-1.934462
30	6	0	4.789390	-0.265602	-2.509273
31	1	0	5.634501	-0.485512	-3.175041
32	1	0	3.974596	0.139450	-3.121954
33	6	0	-2.020207	0.029566	3.436673
34	6	0	-0.752720	-4.400374	-0.638405
35	6	0	-2.666239	-1.329410	3.858231
36	1	0	-1.924595	-1.874104	4.453792
37	1	0	-3.508729	-1.087562	4.519461
38	6	0	-1.605525	-4.950877	0.550880
39	1	0	-2.106923	-5.856957	0.186310
40	1	0	-0.910588	-5.252111	1.343209
41	6	0	-3.119737	-2.193944	2.710799
42	6	0	-2.239707	-3.146368	2.177073
43	6	0	-4.399316	-2.072189	2.146487
44	6	0	-2.605491	-3.970261	1.103359
45	1	0	-1.247124	-3.250550	2.609824
46	6	0	-4.782583	-2.890108	1.080385
47	1	0	-5.101529	-1.351846	2.559202
48	6	0	-3.893283	-3.834680	0.561713

49	1	0	-5.777661	-2.794251	0.655704
50	1	0	-4.201218	-4.481216	-0.257139
51	8	0	-1.052597	1.975133	-3.893817
52	16	0	-0.247458	1.955917	-2.676072
53	8	0	1.195723	2.071424	-2.727103
54	7	0	-0.759881	0.703924	-1.723864
55	8	0	-0.683849	3.234541	-1.746405
56	6	0	-2.988150	1.197866	-0.926373
57	1	0	-1.141418	-0.008104	-2.354855
58	1	0	-2.645432	0.492226	-0.172231
59	6	0	-3.825436	0.642608	-1.928579
60	6	0	-4.483413	1.376562	-2.947144
61	6	0	-3.997765	-0.768143	-1.914952
62	6	0	-5.274746	0.732248	-3.882818
63	1	0	-4.367069	2.456925	-2.997257
64	6	0	-4.789953	-1.402435	-2.853245
65	1	0	-3.481719	-1.342162	-1.142114
66	6	0	-5.435437	-0.655411	-3.843779
67	1	0	-5.771691	1.312490	-4.657946
68	1	0	-4.909303	-2.484908	-2.819823
69	1	0	-6.057857	-1.152413	-4.585505
70	6	0	-2.765330	2.631585	-0.574096
71	1	0	-2.063483	2.623998	0.274783
72	6	0	-4.096054	3.256214	-0.097239
73	6	0	-4.029491	4.691297	0.436019
74	1	0	-4.836723	3.208472	-0.909940
75	1	0	-3.807499	5.369161	-0.404356
76	6	0	3.824636	-2.507510	-3.110372
77	1	0	4.649630	-2.659581	-3.814642
78	1	0	3.492073	-3.491217	-2.761401
79	1	0	2.996805	-2.023344	-3.635084
80	6	0	5.431834	-2.347435	-1.176175
81	1	0	5.092757	-3.312786	-0.789652
82	1	0	6.276408	-2.520436	-1.853054
83	1	0	5.777061	-1.753281	-0.326860
84	6	0	1.450923	3.788448	2.062150
85	1	0	0.840550	3.398530	2.885990
86	1	0	1.802722	4.787558	2.341882
87	1	0	0.823091	3.868388	1.169544
88	6	0	3.546329	2.744613	3.018055
89	1	0	3.927152	3.733202	3.299219
90	1	0	2.985788	2.333203	3.862577
91	1	0	4.394480	2.081151	2.829563
92	6	0	0.369042	-5.408967	-0.938015
93	1	0	-0.067563	-6.384878	-1.177051

94	1	0	0.965551	-5.086322	-1.797720
95	1	0	1.032303	-5.517531	-0.076010
96	6	0	-1.622897	-4.189973	-1.878662
97	1	0	-1.033491	-3.786210	-2.706787
98	1	0	-2.051601	-5.149358	-2.190826
99	1	0	-2.438018	-3.488536	-1.682882
100	6	0	-3.069104	0.967529	2.837224
101	1	0	-3.832293	1.199821	3.589238
102	1	0	-2.606581	1.904529	2.508305
103	1	0	-3.559289	0.515517	1.968798
104	6	0	-1.374249	0.669694	4.677386
105	1	0	-0.937179	1.644150	4.433527
106	1	0	-2.133382	0.822860	5.452213
107	1	0	-0.584628	0.027513	5.076167
108	6	0	-2.089503	3.491764	-1.647712
109	1	0	-2.133387	4.546942	-1.360243
110	1	0	-2.547032	3.388872	-2.639818
111	1	0	-4.498203	2.609214	0.698911
112	6	0	-5.393650	5.084240	0.989113
113	1	0	-5.656652	4.461308	1.855416
114	1	0	-5.406638	6.129887	1.318825
115	1	0	-6.185973	4.958954	0.240828
116	6	0	-2.945268	4.873037	1.489792
117	1	0	-2.961707	5.889485	1.900710
118	1	0	-3.095737	4.177552	2.327893
119	1	0	-1.938885	4.697694	1.090051

R-^{1}PC$_B$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.393127	-1.648147	1.463711
2	45	0	0.369882	-0.161437	-0.149349
3	8	0	2.460339	-0.024581	2.180398
4	6	0	2.303912	1.136064	1.626841
5	8	0	1.501212	1.378298	0.630559
6	8	0	2.886030	-2.045941	0.101705
7	6	0	2.809419	-1.525630	-1.082582
8	8	0	1.852957	-0.736595	-1.476166
9	8	0	-0.765796	-1.729825	-0.871949
10	6	0	-0.565221	-2.920999	-0.387116
11	8	0	0.247523	-3.181045	0.586650
12	8	0	-0.138005	-1.187121	2.795855
13	6	0	-1.037984	-0.323344	2.451024
14	8	0	-1.064324	0.283838	1.302498

15	6	0	3.085392	2.325412	2.160706
16	6	0	3.854856	2.975554	0.966579
17	1	0	3.106931	3.369443	0.268218
18	1	0	4.414045	3.827164	1.376573
19	6	0	4.778576	2.032578	0.242694
20	6	0	4.298675	1.274653	-0.835868
21	6	0	6.112523	1.863791	0.643715
22	6	0	5.109990	0.337231	-1.491646
23	1	0	3.275753	1.418875	-1.177560
24	6	0	6.939804	0.953095	-0.016215
25	1	0	6.501999	2.455927	1.468955
26	6	0	6.441030	0.188605	-1.072983
27	1	0	7.974565	0.839046	0.293253
28	1	0	7.086067	-0.523462	-1.582937
29	6	0	3.891668	-1.849893	-2.101527
30	6	0	4.529042	-0.509714	-2.591772
31	1	0	5.303616	-0.780994	-3.321342
32	1	0	3.750915	0.050524	-3.121757
33	6	0	-2.134024	-0.006717	3.459823
34	6	0	-1.347028	-4.077284	-0.994984
35	6	0	-2.880302	-1.335255	3.802505
36	1	0	-2.169660	-1.989252	4.320569
37	1	0	-3.675365	-1.077773	4.514934
38	6	0	-2.257973	-4.686797	0.118935
39	1	0	-2.853131	-5.476735	-0.357358
40	1	0	-1.604163	-5.165041	0.857649
41	6	0	-3.449742	-2.051271	2.606040
42	6	0	-2.677869	-3.016493	1.944456
43	6	0	-4.734568	-1.769466	2.115542
44	6	0	-3.148547	-3.686891	0.806299
45	1	0	-1.688918	-3.257243	2.328331
46	6	0	-5.223230	-2.434786	0.988643
47	1	0	-5.355673	-1.038630	2.628312
48	6	0	-4.435123	-3.384837	0.333524
49	1	0	-6.223745	-2.217779	0.625401
50	1	0	-4.822496	-3.909824	-0.537179
51	8	0	-0.995719	2.293374	-3.989655
52	16	0	-0.073358	2.007802	-2.904090
53	8	0	1.263076	1.535368	-3.146532
54	7	0	-0.842066	0.944834	-1.771123
55	8	0	0.059883	3.297953	-1.951556
56	6	0	-2.137930	1.464452	-1.168684
57	1	0	-1.062336	0.089790	-2.296370
58	1	0	-2.248738	0.816737	-0.292750
59	6	0	-3.348654	1.182320	-2.026543

60	6	0	-3.836282	2.014575	-3.039055
61	6	0	-4.023117	-0.017877	-1.764355
62	6	0	-4.960237	1.649337	-3.773350
63	1	0	-3.330628	2.948298	-3.272463
64	6	0	-5.141710	-0.388999	-2.504037
65	1	0	-3.657205	-0.667926	-0.964529
66	6	0	-5.613431	0.446681	-3.512256
67	1	0	-5.325743	2.308494	-4.558797
68	1	0	-5.644388	-1.330442	-2.284065
69	1	0	-6.489804	0.164850	-4.093218
70	6	0	-1.903573	2.866260	-0.581138
71	1	0	-1.196622	2.696938	0.247456
72	6	0	-3.196196	3.443405	-0.010407
73	6	0	-3.065552	4.790696	0.709987
74	1	0	-3.942931	3.543648	-0.812289
75	1	0	-2.848074	5.564538	-0.046640
76	6	0	3.220832	-2.528123	-3.310099
77	1	0	3.973127	-2.735306	-4.078997
78	1	0	2.762823	-3.479632	-3.018773
79	1	0	2.449221	-1.880188	-3.736043
80	6	0	4.947820	-2.770936	-1.490466
81	1	0	4.501480	-3.713296	-1.161179
82	1	0	5.717427	-2.991101	-2.239464
83	1	0	5.424289	-2.309511	-0.621837
84	6	0	2.069650	3.353125	2.694876
85	1	0	1.481547	2.933213	3.519053
86	1	0	2.599255	4.236208	3.069137
87	1	0	1.385614	3.661763	1.898662
88	6	0	4.043763	1.894148	3.270199
89	1	0	4.600692	2.765941	3.632861
90	1	0	3.497299	1.455139	4.109364
91	1	0	4.756233	1.146509	2.912507
92	6	0	-0.348565	-5.156186	-1.449278
93	1	0	-0.894461	-6.033036	-1.814485
94	1	0	0.282808	-4.786464	-2.264411
95	1	0	0.296859	-5.458675	-0.620554
96	6	0	-2.192210	-3.605036	-2.179830
97	1	0	-1.563396	-3.170913	-2.962781
98	1	0	-2.732947	-4.458666	-2.604653
99	1	0	-2.919376	-2.844904	-1.880032
100	6	0	-3.107710	1.029621	2.898941
101	1	0	-3.878024	1.256979	3.645323
102	1	0	-2.581493	1.956104	2.648859
103	1	0	-3.598752	0.668604	1.989059
104	6	0	-1.469712	0.527288	4.741421

105	1	0	-0.963306	1.480141	4.549875
106	1	0	-2.230927	0.696394	5.510902
107	1	0	-0.733243	-0.185663	5.120984
108	6	0	-1.215485	3.839206	-1.519453
109	1	0	-0.939330	4.764939	-1.006233
110	1	0	-1.809452	4.102336	-2.405540
111	1	0	-3.616176	2.703264	0.688402
112	6	0	-4.395421	5.144947	1.362700
113	1	0	-4.644991	4.416593	2.147494
114	1	0	-4.364581	6.136505	1.829775
115	1	0	-5.217551	5.140050	0.636624
116	6	0	-1.939676	4.816384	1.737039
117	1	0	-1.914498	5.776392	2.266611
118	1	0	-2.072377	4.029957	2.493830
119	1	0	-0.951987	4.666657	1.284773

A-^{3}TS1$_T$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-3.048079	0.441215	0.277854
2	45	0	-0.703657	0.001398	-0.160333
3	8	0	-3.008042	1.878090	-1.192752
4	6	0	-1.908363	2.107851	-1.835752
5	8	0	-0.794881	1.469154	-1.614816
6	8	0	-2.491715	1.842541	1.689995
7	6	0	-1.230895	2.029315	1.921743
8	8	0	-0.276854	1.401139	1.297713
9	8	0	-0.796123	-1.440632	1.354249
10	6	0	-1.893627	-1.600988	2.028286
11	8	0	-3.007392	-0.990003	1.761033
12	8	0	-3.498713	-0.976506	-1.169584
13	6	0	-2.547634	-1.579797	-1.813535
14	8	0	-1.282110	-1.394858	-1.583220
15	6	0	-1.888571	3.161568	-2.928796
16	6	0	-0.749960	4.183267	-2.609069
17	1	0	0.205572	3.650093	-2.673241
18	1	0	-0.770170	4.933744	-3.410249
19	6	0	-0.878117	4.839014	-1.259667
20	6	0	-0.275017	4.246245	-0.141071
21	6	0	-1.621607	6.015436	-1.081326
22	6	0	-0.432719	4.782372	1.145396
23	1	0	0.341221	3.359589	-0.270979
24	6	0	-1.763552	6.576056	0.189850
25	1	0	-2.079822	6.495558	-1.943121

26	6	0	-1.179847	5.959902	1.298828
27	1	0	-2.328546	7.494862	0.316085
28	1	0	-1.294115	6.396970	2.288095
29	6	0	-0.794617	3.020231	2.986595
30	6	0	0.165595	4.062039	2.323940
31	1	0	0.446410	4.771380	3.113471
32	1	0	1.071892	3.529551	2.011441
33	6	0	-2.950331	-2.579618	-2.885631
34	6	0	-1.904879	-2.585094	3.186642
35	6	0	-3.246114	3.858719	-3.022375
36	1	0	-3.208966	4.622186	-3.807716
37	1	0	-4.036946	3.144482	-3.267455
38	1	0	-3.513259	4.338705	-2.077477
39	6	0	-1.553168	2.456301	-4.257207
40	1	0	-2.330932	1.731135	-4.522189
41	1	0	-1.494871	3.199033	-5.060066
42	1	0	-0.595244	1.933508	-4.188101
43	6	0	0.002515	2.244305	4.052942
44	1	0	0.379549	2.944221	4.806379
45	1	0	-0.634852	1.511657	4.560091
46	1	0	0.848929	1.720427	3.600012
47	6	0	-2.010640	3.702699	3.612051
48	1	0	-2.666005	2.970061	4.091454
49	1	0	-1.675652	4.420239	4.369739
50	1	0	-2.600605	4.233620	2.860554
51	6	0	-3.683579	-3.764452	-2.174039
52	1	0	-4.654956	-3.390758	-1.829942
53	1	0	-3.873764	-4.524430	-2.943060
54	6	0	-3.940716	-1.897430	-3.845570
55	1	0	-4.797306	-1.493493	-3.300306
56	1	0	-3.457739	-1.077323	-4.387920
57	1	0	-4.298882	-2.625768	-4.581144
58	6	0	-2.814994	-3.787264	2.765302
59	1	0	-2.710560	-4.551102	3.546673
60	1	0	-3.853280	-3.436049	2.782877
61	6	0	-2.537381	-1.900597	4.410385
62	1	0	-1.906188	-1.081756	4.771291
63	1	0	-3.522098	-1.495738	4.165094
64	1	0	-2.643136	-2.629369	5.221364
65	6	0	-0.493033	-3.064668	3.522669
66	1	0	-0.527347	-3.681583	4.427659
67	1	0	-0.069137	-3.661893	2.712586
68	1	0	0.181849	-2.220863	3.697374
69	6	0	-1.729496	-3.081844	-3.656659
70	1	0	-1.031591	-3.610252	-3.003283

71	1	0	-2.057058	-3.766392	-4.447451
72	1	0	-1.186124	-2.251598	-4.117395
73	6	0	-2.932961	-4.352346	-1.007639
74	6	0	-3.192413	-3.874877	0.284865
75	6	0	-1.957325	-5.348579	-1.169730
76	6	0	-2.505021	-4.360032	1.406916
77	1	0	-3.951993	-3.107789	0.421996
78	6	0	-1.259415	-5.839711	-0.063622
79	1	0	-1.754546	-5.746594	-2.161327
80	6	0	-1.529684	-5.351154	1.217038
81	1	0	-0.507657	-6.611828	-0.199250
82	1	0	-0.995755	-5.752108	2.075528
83	8	0	2.642711	0.113967	1.697225
84	16	0	2.450183	0.504288	0.302821
85	8	0	2.344122	1.901924	-0.066462
86	7	0	1.243652	-0.362497	-0.401719
87	6	0	4.338880	-1.317690	-0.194240
88	6	0	3.671857	-2.438241	-0.984659
89	6	0	2.248078	-2.758329	-0.587288
90	1	0	3.716037	-2.174345	-2.051044
91	1	0	4.287896	-3.347162	-0.864100
92	1	0	1.677380	-1.580374	-0.518103
93	8	0	3.737096	-0.042781	-0.557246
94	1	0	4.198031	-1.458316	0.887279
95	6	0	1.421783	-3.440291	-1.642156
96	1	0	0.374269	-3.510118	-1.325336
97	1	0	1.454122	-2.902424	-2.597739
98	1	0	1.784396	-4.467003	-1.821440
99	6	0	2.053730	-3.310684	0.799043
100	1	0	0.984529	-3.403008	1.015834
101	1	0	2.504667	-4.313744	0.884253
102	1	0	2.494438	-2.674256	1.576785
103	6	0	5.815800	-1.175811	-0.507298
104	1	0	5.938578	-0.991366	-1.585238
105	1	0	6.303498	-2.140798	-0.304066
106	6	0	6.506084	-0.068925	0.288038
107	1	0	5.999227	0.881943	0.079646
108	1	0	6.373858	-0.262955	1.362937
109	6	0	7.966665	0.030242	-0.049446
110	6	0	8.398017	0.824460	-1.116305
111	6	0	8.920917	-0.710925	0.653632
112	6	0	9.742744	0.878753	-1.470282
113	1	0	7.664433	1.410375	-1.671879
114	6	0	10.267399	-0.659784	0.304499
115	1	0	8.600391	-1.332430	1.491352

116	6	0	10.682793	0.135574	-0.760448
117	1	0	10.058329	1.507112	-2.301846
118	1	0	10.995765	-1.240370	0.868861
119	1	0	11.735558	0.178628	-1.034009

A-^{1}TS1$_{T}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-3.037323	0.402146	0.291944
2	45	0	-0.683676	-0.027673	-0.146492
3	8	0	-3.062510	1.835204	-1.173293
4	6	0	-1.973981	2.059819	-1.837432
5	8	0	-0.852337	1.434029	-1.633918
6	8	0	-2.477541	1.805100	1.704173
7	6	0	-1.217821	1.993547	1.933563
8	8	0	-0.259010	1.375738	1.305214
9	8	0	-0.731254	-1.434763	1.370870
10	6	0	-1.825124	-1.614415	2.050801
11	8	0	-2.947844	-1.028710	1.779640
12	8	0	-3.481926	-1.023728	-1.153777
13	6	0	-2.528007	-1.619068	-1.798425
14	8	0	-1.261578	-1.435432	-1.570483
15	6	0	-1.982296	3.109498	-2.936293
16	6	0	-0.872696	4.161706	-2.614316
17	1	0	0.096991	3.655562	-2.684827
18	1	0	-0.916459	4.916039	-3.411008
19	6	0	-1.011847	4.806713	-1.260662
20	6	0	-0.381574	4.228191	-0.149691
21	6	0	-1.785480	5.961838	-1.071310
22	6	0	-0.533026	4.761061	1.138916
23	1	0	0.252331	3.355342	-0.288909
24	6	0	-1.929339	6.514997	0.202948
25	1	0	-2.265239	6.431778	-1.926924
26	6	0	-1.312750	5.915827	1.303507
27	1	0	-2.520161	7.416194	0.337994
28	1	0	-1.425114	6.349758	2.294456
29	6	0	-0.781444	2.988302	2.995157
30	6	0	0.117499	4.067592	2.306055
31	1	0	0.389704	4.790490	3.086316
32	1	0	1.035086	3.568171	1.973241
33	6	0	-2.932118	-2.624102	-2.866652
34	6	0	-1.809005	-2.597630	3.208529
35	6	0	-3.356976	3.771686	-3.033340

36	1	0	-3.337713	4.535322	-3.819399
37	1	0	-4.128968	3.037296	-3.279473
38	1	0	-3.638646	4.244539	-2.089122
39	6	0	-1.624626	2.412626	-4.262292
40	1	0	-2.384552	1.669743	-4.530032
41	1	0	-1.578946	3.155516	-5.066015
42	1	0	-0.656101	1.910789	-4.186744
43	6	0	0.081211	2.236848	4.026976
44	1	0	0.453142	2.944647	4.775826
45	1	0	-0.507347	1.472532	4.546784
46	1	0	0.933215	1.751238	3.541926
47	6	0	-1.998502	3.623111	3.666521
48	1	0	-2.611426	2.863552	4.160491
49	1	0	-1.664250	4.346092	4.419401
50	1	0	-2.632918	4.137248	2.940232
51	6	0	-3.624707	-3.825261	-2.139842
52	1	0	-4.599767	-3.474470	-1.782332
53	1	0	-3.807407	-4.593164	-2.902879
54	6	0	-3.957113	-1.963706	-3.803965
55	1	0	-4.805773	-1.572358	-3.237762
56	1	0	-3.502028	-1.136339	-4.359278
57	1	0	-4.320966	-2.699907	-4.528997
58	6	0	-2.697435	-3.817070	2.790306
59	1	0	-2.572829	-4.580910	3.568792
60	1	0	-3.742258	-3.486597	2.815404
61	6	0	-2.447275	-1.925690	4.435927
62	1	0	-1.831986	-1.091714	4.789838
63	1	0	-3.442169	-1.542753	4.196340
64	1	0	-2.531547	-2.654571	5.249334
65	6	0	-0.385687	-3.049508	3.534639
66	1	0	-0.400887	-3.668995	4.438392
67	1	0	0.045222	-3.636196	2.720181
68	1	0	0.271386	-2.191442	3.707443
69	6	0	-1.719126	-3.102327	-3.664501
70	1	0	-1.009396	-3.639158	-3.031007
71	1	0	-2.052481	-3.774814	-4.463263
72	1	0	-1.187855	-2.259348	-4.116278
73	6	0	-2.844109	-4.390333	-0.981630
74	6	0	-3.096663	-3.913412	0.312706
75	6	0	-1.849443	-5.366249	-1.152521
76	6	0	-2.386523	-4.381250	1.428147
77	1	0	-3.869456	-3.160726	0.456195
78	6	0	-1.127080	-5.838346	-0.053670
79	1	0	-1.653197	-5.765741	-2.144838
80	6	0	-1.392577	-5.352140	1.229062

81	1	0	-0.363667	-6.597926	-0.195508
82	1	0	-0.842542	-5.741755	2.082647
83	8	0	2.435296	0.046699	1.643722
84	16	0	2.372912	0.548324	0.274928
85	8	0	2.272498	1.967735	-0.008539
86	7	0	1.237088	-0.199151	-0.692025
87	6	0	4.340930	-1.189929	-0.174268
88	6	0	3.648689	-2.255602	-1.015997
89	6	0	2.219144	-2.576490	-0.643813
90	1	0	3.701737	-1.948138	-2.069798
91	1	0	4.231366	-3.189420	-0.931999
92	1	0	1.647479	-1.453250	-0.672928
93	8	0	3.770273	0.107594	-0.473577
94	1	0	4.204273	-1.380820	0.901021
95	6	0	1.438454	-3.290792	-1.713049
96	1	0	0.392856	-3.412322	-1.411669
97	1	0	1.466039	-2.754502	-2.668662
98	1	0	1.863876	-4.295398	-1.873305
99	6	0	2.003901	-3.122552	0.739691
100	1	0	0.940822	-3.312147	0.910486
101	1	0	2.544494	-4.078311	0.841832
102	1	0	2.356422	-2.446708	1.526658
103	6	0	5.817538	-1.069642	-0.500246
104	1	0	5.928174	-0.844070	-1.571617
105	1	0	6.286427	-2.052495	-0.343451
106	6	0	6.546005	-0.011060	0.326032
107	1	0	6.049769	0.955739	0.174064
108	1	0	6.439905	-0.251928	1.394118
109	6	0	7.999001	0.080941	-0.045241
110	6	0	8.410344	0.887014	-1.111309
111	6	0	8.964049	-0.675449	0.625593
112	6	0	9.746821	0.938056	-1.495354
113	1	0	7.667879	1.484955	-1.641816
114	6	0	10.302610	-0.627458	0.246263
115	1	0	8.658811	-1.305830	1.462346
116	6	0	10.698226	0.179829	-0.817044
117	1	0	10.047346	1.575700	-2.325405
118	1	0	11.040332	-1.219371	0.786152
119	1	0	11.744742	0.220846	-1.113752

A-^{3}IM2$_T$

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

1	45	0	-2.868653	0.258155	0.870414
2	45	0	-0.720932	0.016396	-0.226620
3	8	0	-3.395396	1.631158	-0.576849
4	6	0	-2.574426	1.906834	-1.538341
5	8	0	-1.388455	1.377181	-1.654226
6	8	0	-2.066730	1.760589	2.042158
7	6	0	-0.817760	2.070428	1.889203
8	8	0	-0.037818	1.511450	1.011497
9	8	0	-0.217026	-1.355963	1.222554
10	6	0	-1.038133	-1.621374	2.189456
11	8	0	-2.229922	-1.109060	2.285058
12	8	0	-3.567984	-1.254278	-0.363869
13	6	0	-2.789459	-1.802349	-1.247207
14	8	0	-1.541380	-1.481729	-1.405820
15	6	0	-2.995000	2.899953	-2.607944
16	6	0	-1.948089	4.060428	-2.632140
17	1	0	-0.995475	3.644678	-2.979712
18	1	0	-2.294119	4.776579	-3.388807
19	6	0	-1.753168	4.742450	-1.303737
20	6	0	-0.784434	4.263181	-0.409795
21	6	0	-2.542173	5.836937	-0.919063
22	6	0	-0.611482	4.832973	0.860353
23	1	0	-0.141648	3.438653	-0.710925
24	6	0	-2.366598	6.429331	0.333204
25	1	0	-3.284821	6.230753	-1.609182
26	6	0	-1.412001	5.927928	1.220437
27	1	0	-2.971741	7.285203	0.616179
28	1	0	-1.275897	6.392570	2.194110
29	6	0	-0.186672	3.141979	2.757533
30	6	0	0.395884	4.243114	1.811268
31	1	0	0.818246	5.020424	2.461363
32	1	0	1.220268	3.791691	1.247837
33	6	0	-3.377626	-2.889744	-2.130146
34	6	0	-0.584034	-2.593874	3.263344
35	6	0	-4.399119	3.434522	-2.323920
36	1	0	-4.675560	4.156610	-3.100712
37	1	0	-5.134722	2.625365	-2.324462
38	1	0	-4.449763	3.928473	-1.350568
39	6	0	-2.961910	2.182874	-3.970711
40	1	0	-3.696886	1.370934	-4.004633
41	1	0	-3.209030	2.896331	-4.764144
42	1	0	-1.970744	1.765593	-4.168285
43	6	0	0.985849	2.498971	3.523835
44	1	0	1.513406	3.270806	4.094450
45	1	0	0.624191	1.744682	4.231463

46	1	0	1.688043	2.023398	2.832563
47	6	0	-1.215012	3.724925	3.726277
48	1	0	-1.606695	2.951670	4.393223
49	1	0	-0.739360	4.501807	4.335390
50	1	0	-2.062895	4.164009	3.194128
51	6	0	-3.884588	-4.039046	-1.199942
52	1	0	-4.729634	-3.649013	-0.620973
53	1	0	-4.269583	-4.828687	-1.858400
54	6	0	-4.585585	-2.302058	-2.882164
55	1	0	-5.316550	-1.888286	-2.182686
56	1	0	-4.271286	-1.508493	-3.568772
57	1	0	-5.066577	-3.088673	-3.473358
58	6	0	-1.557860	-3.816248	3.246950
59	1	0	-1.180289	-4.529112	3.991224
60	1	0	-2.537624	-3.465070	3.591563
61	6	0	-0.698680	-1.892551	4.628814
62	1	0	-0.002708	-1.049468	4.693727
63	1	0	-1.713487	-1.520326	4.793203
64	1	0	-0.446882	-2.601448	5.424938
65	6	0	0.858014	-3.039802	3.012832
66	1	0	1.181182	-3.695061	3.829849
67	1	0	0.949890	-3.584504	2.069460
68	1	0	1.532259	-2.179558	2.962041
69	6	0	-2.337114	-3.411893	-3.122119
70	1	0	-1.465407	-3.828048	-2.609262
71	1	0	-2.788001	-4.195434	-3.741711
72	1	0	-1.983891	-2.611663	-3.779320
73	6	0	-2.836862	-4.586018	-0.266514
74	6	0	-2.687970	-4.029599	1.011621
75	6	0	-1.979568	-5.628911	-0.649182
76	6	0	-1.699263	-4.476238	1.900491
77	1	0	-3.360095	-3.232716	1.323192
78	6	0	-0.995442	-6.091535	0.227123
79	1	0	-2.094202	-6.084310	-1.629913
80	6	0	-0.852185	-5.517749	1.492532
81	1	0	-0.342684	-6.905330	-0.074046
82	1	0	-0.089950	-5.886669	2.174736
83	8	0	2.582785	0.117253	0.829267
84	16	0	2.428703	0.663010	-0.508553
85	8	0	2.522646	2.094614	-0.750455
86	7	0	1.082501	0.002281	-1.189599
87	6	0	4.200009	-1.231243	-1.127009
88	6	0	3.740623	-2.299451	-2.120384
89	6	0	2.284616	-2.616134	-2.056600
90	1	0	4.029021	-1.979207	-3.131911

91	1	0	4.343964	-3.199641	-1.896373
92	1	0	1.000014	0.359021	-2.146961
93	8	0	3.597576	0.047265	-1.479837
94	1	0	3.868894	-1.490766	-0.111821
95	6	0	1.411112	-2.448926	-3.245262
96	1	0	0.411410	-2.096389	-2.952875
97	1	0	1.834489	-1.740945	-3.970547
98	1	0	1.251079	-3.399025	-3.789153
99	6	0	1.720898	-3.152509	-0.789155
100	1	0	0.671218	-3.453910	-0.899557
101	1	0	2.287117	-4.023638	-0.416335
102	1	0	1.733942	-2.402022	0.019602
103	6	0	5.700120	-1.003098	-1.132028
104	1	0	6.015588	-0.699039	-2.141716
105	1	0	6.197458	-1.963678	-0.930941
106	6	0	6.150854	0.042299	-0.112034
107	1	0	5.619601	0.981282	-0.319294
108	1	0	5.835884	-0.273892	0.893028
109	6	0	7.635036	0.271196	-0.143644
110	6	0	8.208242	1.060733	-1.146728
111	6	0	8.481622	-0.319414	0.797885
112	6	0	9.583915	1.256513	-1.205667
113	1	0	7.559005	1.534204	-1.884761
114	6	0	9.859556	-0.125512	0.744836
115	1	0	8.049372	-0.934547	1.588549
116	6	0	10.415648	0.663574	-0.258160
117	1	0	10.008930	1.881148	-1.990193
118	1	0	10.500897	-0.589199	1.493068
119	1	0	11.492324	0.819882	-0.299467

A-^{3}TS2$_T$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-2.934686	-0.061654	0.854770
2	45	0	-0.731827	-0.004607	-0.213504
3	8	0	-3.586513	1.253231	-0.601997
4	6	0	-2.784052	1.654148	-1.536230
5	8	0	-1.542668	1.273760	-1.638180
6	8	0	-2.362150	1.536051	2.037726
7	6	0	-1.168905	2.026422	1.899831
8	8	0	-0.302964	1.570642	1.046986
9	8	0	-0.068689	-1.305040	1.243230
10	6	0	-0.866385	-1.690622	2.187539

11	8	0	-2.118199	-1.346362	2.266594
12	8	0	-3.412720	-1.643472	-0.398213
13	6	0	-2.563661	-2.085541	-1.276508
14	8	0	-1.364327	-1.613066	-1.419579
15	6	0	-3.302841	2.607938	-2.600063
16	6	0	-2.355301	3.849193	-2.660497
17	1	0	-1.369501	3.501713	-2.990465
18	1	0	-2.754562	4.508789	-3.442353
19	6	0	-2.227275	4.590891	-1.355810
20	6	0	-1.253034	4.199693	-0.424876
21	6	0	-3.086429	5.650589	-1.027735
22	6	0	-1.153342	4.812993	0.832760
23	1	0	-0.548676	3.412631	-0.683937
24	6	0	-2.977925	6.292168	0.207864
25	1	0	-3.832888	5.976525	-1.748641
26	6	0	-2.024579	5.869877	1.136515
27	1	0	-3.636636	7.121677	0.446852
28	1	0	-1.944670	6.366661	2.100662
29	6	0	-0.710421	3.181362	2.770227
30	6	0	-0.153095	4.304812	1.836515
31	1	0	0.181727	5.118126	2.493543
32	1	0	0.726847	3.905271	1.319148
33	6	0	-3.019259	-3.229988	-2.167693
34	6	0	-0.313362	-2.612296	3.261566
35	6	0	-4.740130	3.029432	-2.293480
36	1	0	-5.095220	3.706704	-3.078656
37	1	0	-5.403394	2.161269	-2.254529
38	1	0	-4.808335	3.543543	-1.331482
39	6	0	-3.238641	1.879001	-3.956850
40	1	0	-3.899036	1.004573	-3.964893
41	1	0	-3.566138	2.558290	-4.751277
42	1	0	-2.218629	1.549294	-4.174300
43	6	0	0.449336	2.667603	3.647253
44	1	0	0.842440	3.494344	4.248935
45	1	0	0.105100	1.884531	4.331866
46	1	0	1.255350	2.264546	3.026902
47	6	0	-1.857170	3.694744	3.640394
48	1	0	-2.225759	2.909446	4.306175
49	1	0	-1.501979	4.531938	4.252278
50	1	0	-2.698580	4.038739	3.032966
51	6	0	-3.366117	-4.444539	-1.246856
52	1	0	-4.255196	-4.175393	-0.665384
53	1	0	-3.641382	-5.274438	-1.910641
54	6	0	-4.298918	-2.794449	-2.903752
55	1	0	-5.071223	-2.488976	-2.193191

56	1	0	-4.095952	-1.955943	-3.578741
57	1	0	-4.678867	-3.628534	-3.503733
58	6	0	-1.122605	-3.949132	3.216971
59	1	0	-0.668550	-4.615522	3.961823
60	1	0	-2.144394	-3.729919	3.548156
61	6	0	-0.539787	-1.949793	4.632285
62	1	0	0.043098	-1.026997	4.718680
63	1	0	-1.596151	-1.710447	4.781133
64	1	0	-0.215281	-2.631686	5.425799
65	6	0	1.177202	-2.870716	3.035651
66	1	0	1.562543	-3.504594	3.842719
67	1	0	1.353147	-3.372365	2.080224
68	1	0	1.740090	-1.933088	3.024571
69	6	0	-1.932348	-3.607898	-3.174053
70	1	0	-1.014845	-3.926910	-2.671424
71	1	0	-2.289398	-4.430266	-3.804823
72	1	0	-1.682957	-2.761143	-3.820632
73	6	0	-2.255823	-4.850908	-0.314589
74	6	0	-2.193297	-4.292590	0.969939
75	6	0	-1.259451	-5.760809	-0.700009
76	6	0	-1.159770	-4.608323	1.863568
77	1	0	-2.972176	-3.601900	1.285506
78	6	0	-0.228465	-6.094175	0.181305
79	1	0	-1.304561	-6.219328	-1.685120
80	6	0	-0.174703	-5.519858	1.453419
81	1	0	0.530774	-6.809355	-0.121186
82	1	0	0.624178	-5.789392	2.140216
83	8	0	2.517429	0.449305	0.938616
84	16	0	2.328511	1.004371	-0.392284
85	8	0	2.164729	2.435232	-0.595073
86	7	0	1.198387	0.090112	-1.173067
87	6	0	4.292844	-0.619494	-1.089210
88	6	0	3.779904	-1.586592	-2.160739
89	6	0	2.364379	-2.024375	-2.022467
90	1	0	3.952235	-1.131560	-3.145957
91	1	0	4.433909	-2.478274	-2.111506
92	1	0	1.055902	0.539529	-2.086032
93	8	0	3.692379	0.678252	-1.271097
94	1	0	4.027959	-0.984059	-0.086138
95	6	0	1.490796	-2.086044	-3.216630
96	1	0	0.447036	-1.881016	-2.943116
97	1	0	1.808339	-1.389804	-4.002453
98	1	0	1.497080	-3.098425	-3.660313
99	6	0	1.947922	-2.751827	-0.797677
100	1	0	0.862599	-2.899581	-0.758001

101	1	0	2.426331	-3.746900	-0.749281
102	1	0	2.229442	-2.211059	0.115686
103	6	0	5.792651	-0.404874	-1.163887
104	1	0	6.051551	0.023022	-2.144168
105	1	0	6.287844	-1.386347	-1.114233
106	6	0	6.316621	0.497559	-0.047322
107	1	0	5.811575	1.469318	-0.116855
108	1	0	6.025484	0.067309	0.922598
109	6	0	7.807110	0.670725	-0.114416
110	6	0	8.373489	1.714852	-0.851808
111	6	0	8.664664	-0.237169	0.514562
112	6	0	9.754724	1.850375	-0.956552
113	1	0	7.716661	2.433172	-1.344280
114	6	0	10.046501	-0.106421	0.413584
115	1	0	8.237420	-1.055048	1.097285
116	6	0	10.596659	0.939172	-0.323957
117	1	0	10.175795	2.674597	-1.530497
118	1	0	10.696718	-0.821004	0.916454
119	1	0	11.677248	1.045740	-0.401498

A-^{1}PC$_{T}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-3.087444	0.190588	0.370472
2	45	0	-0.736100	-0.054573	-0.145582
3	8	0	-3.163829	1.588698	-1.161926
4	6	0	-2.108295	1.899328	-1.838712
5	8	0	-0.932113	1.364952	-1.647217
6	8	0	-2.592306	1.666073	1.720525
7	6	0	-1.343861	1.934977	1.934512
8	8	0	-0.358760	1.378352	1.294243
9	8	0	-0.626667	-1.448995	1.361578
10	6	0	-1.660683	-1.702984	2.098778
11	8	0	-2.843952	-1.197999	1.908808
12	8	0	-3.531255	-1.300726	-1.009342
13	6	0	-2.557760	-1.843363	-1.669704
14	8	0	-1.307109	-1.536959	-1.507003
15	6	0	-2.217460	2.945819	-2.936556
16	6	0	-1.207117	4.094342	-2.618886
17	1	0	-0.196004	3.676998	-2.695017
18	1	0	-1.319189	4.840317	-3.416923
19	6	0	-1.391659	4.730265	-1.266205

20	6	0	-0.710243	4.212872	-0.155563
21	6	0	-2.253013	5.822029	-1.078362
22	6	0	-0.889735	4.742782	1.130582
23	1	0	-0.017557	3.384768	-0.289013
24	6	0	-2.429556	6.371868	0.193247
25	1	0	-2.775811	6.246139	-1.932735
26	6	0	-1.757920	5.832839	1.292820
27	1	0	-3.090322	7.223278	0.327065
28	1	0	-1.895983	6.264135	2.281623
29	6	0	-0.973077	2.962616	2.991017
30	6	0	-0.175317	4.112920	2.295851
31	1	0	0.036626	4.860454	3.071645
32	1	0	0.780447	3.695577	1.960272
33	6	0	-2.905324	-2.925134	-2.684466
34	6	0	-1.470445	-2.676475	3.251141
35	6	0	-3.644540	3.485885	-3.031899
36	1	0	-3.695804	4.244314	-3.821786
37	1	0	-4.350769	2.685970	-3.270900
38	1	0	-3.963478	3.937259	-2.089357
39	6	0	-1.804291	2.291470	-4.268229
40	1	0	-2.505910	1.497829	-4.548357
41	1	0	-1.808235	3.043558	-5.064908
42	1	0	-0.801587	1.859375	-4.195083
43	6	0	-0.038460	2.280475	4.007877
44	1	0	0.311476	3.018100	4.738525
45	1	0	-0.563604	1.487878	4.551910
46	1	0	0.826389	1.841457	3.501775
47	6	0	-2.224507	3.500916	3.683714
48	1	0	-2.778353	2.694323	4.172219
49	1	0	-1.932959	4.234896	4.443985
50	1	0	-2.900452	3.980440	2.971106
51	6	0	-3.527723	-4.131400	-1.908643
52	1	0	-4.500181	-3.805664	-1.521509
53	1	0	-3.712874	-4.920776	-2.649218
54	6	0	-3.967845	-2.374000	-3.649747
55	1	0	-4.844283	-2.021746	-3.100130
56	1	0	-3.569524	-1.538507	-4.235660
57	1	0	-4.276837	-3.160775	-4.346688
58	6	0	-2.338992	-3.942040	2.959449
59	1	0	-2.122580	-4.665825	3.756143
60	1	0	-3.391750	-3.650192	3.052950
61	6	0	-1.984354	-2.022148	4.544317
62	1	0	-1.371818	-1.155569	4.814057
63	1	0	-3.019731	-1.691179	4.427070
64	1	0	-1.931642	-2.742833	5.367973

65	6	0	0.007118	-3.051126	3.392297
66	1	0	0.134514	-3.719870	4.251793
67	1	0	0.376843	-3.553765	2.494448
68	1	0	0.624270	-2.159833	3.542187
69	6	0	-1.661132	-3.364798	-3.458100
70	1	0	-0.879636	-3.732580	-2.786439
71	1	0	-1.929575	-4.162783	-4.160076
72	1	0	-1.243768	-2.530396	-4.031201
73	6	0	-2.683821	-4.647140	-0.774151
74	6	0	-2.880623	-4.133050	0.514876
75	6	0	-1.686696	-5.615910	-0.966111
76	6	0	-2.104160	-4.552773	1.603781
77	1	0	-3.657877	-3.388181	0.674751
78	6	0	-0.905385	-6.046718	0.108662
79	1	0	-1.535519	-6.041731	-1.955289
80	6	0	-1.109731	-5.518197	1.385515
81	1	0	-0.144000	-6.805366	-0.046217
82	1	0	-0.508860	-5.866092	2.222454
83	8	0	2.388394	-0.139377	1.605512
84	16	0	2.500758	0.722541	0.450547
85	8	0	2.214536	2.135196	0.457819
86	7	0	1.574300	0.013400	-0.814341
87	6	0	4.457966	-0.716696	-0.475478
88	6	0	3.649782	-1.149547	-1.678690
89	6	0	2.130458	-1.249256	-1.463740
90	1	0	3.858721	-0.434580	-2.488970
91	1	0	4.002814	-2.129673	-2.026785
92	1	0	1.475199	0.749136	-1.521152
93	8	0	4.016845	0.634211	-0.132366
94	1	0	4.272245	-1.358355	0.400053
95	6	0	1.461191	-1.327470	-2.829506
96	1	0	0.374343	-1.375863	-2.733656
97	1	0	1.732068	-0.462901	-3.451253
98	1	0	1.803143	-2.229897	-3.351004
99	6	0	1.757291	-2.446596	-0.599001
100	1	0	0.670069	-2.536026	-0.511392
101	1	0	2.144059	-3.363956	-1.060447
102	1	0	2.160826	-2.369145	0.416436
103	6	0	5.941974	-0.617514	-0.752583
104	1	0	6.097505	0.022509	-1.633982
105	1	0	6.299568	-1.618617	-1.034542
106	6	0	6.761550	-0.084462	0.421403
107	1	0	6.389882	0.914706	0.683495
108	1	0	6.590657	-0.719392	1.302544
109	6	0	8.228833	-0.030880	0.099865

110	6	0	8.734605	0.961454	-0.746821
111	6	0	9.112510	-0.990667	0.599025
112	6	0	10.083784	0.993832	-1.084006
113	1	0	8.058053	1.721895	-1.140070
114	6	0	10.464575	-0.961377	0.266594
115	1	0	8.733172	-1.768238	1.263431
116	6	0	10.954230	0.030701	-0.577680
117	1	0	10.458845	1.776977	-1.741237
118	1	0	11.138188	-1.715136	0.671197
119	1	0	12.010654	0.056637	-0.838474

R-^{3}IM1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.219088	1.374265	1.388436
2	45	0	-0.370190	-0.052215	-0.381791
3	8	0	-2.473510	-0.135502	2.015039
4	6	0	-2.434366	-1.266916	1.384164
5	8	0	-1.663070	-1.499041	0.361571
6	8	0	-2.663839	2.040483	0.082233
7	6	0	-2.717260	1.574910	-1.124615
8	8	0	-1.875182	0.698787	-1.596567
9	8	0	0.846724	1.503994	-0.977868
10	6	0	0.802343	2.639182	-0.344142
11	8	0	0.040765	2.854625	0.684516
12	8	0	0.251169	0.645170	2.657626
13	6	0	1.094795	-0.222911	2.183951
14	8	0	1.085281	-0.646366	0.959318
15	6	0	-3.306000	-2.422385	1.840511
16	6	0	-4.122202	-2.938315	0.610738
17	1	0	-3.408423	-3.343819	-0.115828
18	1	0	-4.738746	-3.771021	0.972846
19	6	0	-4.978479	-1.884281	-0.039204
20	6	0	-4.445711	-1.084796	-1.061302
21	6	0	-6.295835	-1.646828	0.381807
22	6	0	-5.181487	-0.037113	-1.634191
23	1	0	-3.440154	-1.287828	-1.423096
24	6	0	-7.051045	-0.625665	-0.198526
25	1	0	-6.729197	-2.271369	1.159469
26	6	0	-6.495246	0.181851	-1.192725
27	1	0	-8.073860	-0.458265	0.125116
28	1	0	-7.083216	0.980964	-1.638255

29	6	0	-3.789286	2.081162	-2.072037
30	6	0	-4.542516	0.850213	-2.669707
31	1	0	-5.299451	1.250704	-3.356313
32	1	0	-3.823965	0.275436	-3.264936
33	6	0	2.161983	-0.780788	3.110237
34	6	0	1.677184	3.778172	-0.833619
35	6	0	-4.228105	-1.984775	2.978471
36	1	0	-4.850399	-2.832923	3.285163
37	1	0	-3.650372	-1.648498	3.843527
38	1	0	-4.881828	-1.163161	2.674895
39	6	0	-2.367832	-3.553287	2.308269
40	1	0	-1.780903	-3.239465	3.178277
41	1	0	-2.966455	-4.422845	2.599219
42	1	0	-1.680624	-3.844500	1.509391
43	6	0	-3.084493	2.829966	-3.220967
44	1	0	-3.833382	3.174895	-3.941543
45	1	0	-2.548294	3.707937	-2.844338
46	1	0	-2.373800	2.177627	-3.736059
47	6	0	-4.753902	3.017334	-1.342158
48	1	0	-4.226656	3.883368	-0.933401
49	1	0	-5.513842	3.373449	-2.046778
50	1	0	-5.256215	2.510403	-0.514336
51	6	0	3.050590	0.407641	3.598332
52	1	0	2.428808	1.049978	4.233039
53	1	0	3.832778	-0.028428	4.232900
54	6	0	1.460709	-1.407496	4.328984
55	1	0	0.815462	-0.679239	4.827494
56	1	0	0.853154	-2.267646	4.028778
57	1	0	2.215422	-1.758319	5.040746
58	6	0	2.617590	4.203585	0.340786
59	1	0	3.258912	5.005040	-0.048260
60	1	0	1.990418	4.634507	1.129900
61	6	0	0.759306	4.966099	-1.179915
62	1	0	0.095334	4.716886	-2.014487
63	1	0	0.147874	5.251866	-0.319899
64	1	0	1.371900	5.822839	-1.479370
65	6	0	2.487735	3.356003	-2.059567
66	1	0	3.088553	4.204585	-2.405186
67	1	0	3.159450	2.524478	-1.831291
68	1	0	1.833534	3.037029	-2.875384
69	6	0	3.005987	-1.832079	2.385153
70	1	0	3.532634	-1.397494	1.529691
71	1	0	3.748358	-2.244134	3.078009
72	1	0	2.376784	-2.647716	2.015710
73	6	0	3.657371	1.222938	2.487308

74	6	0	2.946694	2.313185	1.965160
75	6	0	4.907107	0.909094	1.932315
76	6	0	3.446888	3.080043	0.902970
77	1	0	1.985578	2.576722	2.402371
78	6	0	5.427080	1.673593	0.885950
79	1	0	5.474456	0.069168	2.326558
80	6	0	4.702628	2.750309	0.371011
81	1	0	6.398181	1.427131	0.467826
82	1	0	5.112608	3.342952	-0.443268
83	8	0	-0.350635	-3.687855	-2.287070
84	16	0	0.555360	-2.955122	-1.423696
85	8	0	0.736725	-3.350250	-0.032747
86	7	0	0.301999	-1.361660	-1.643313
87	6	0	3.197755	-3.062231	-1.374423
88	1	0	2.952313	-2.968030	-0.309626
89	8	0	2.034111	-3.118941	-2.175881
90	1	0	3.758095	-3.990184	-1.535901
91	6	0	4.095969	-1.893574	-1.777373
92	17	0	4.522641	-2.007815	-3.504594
93	17	0	5.591828	-2.058728	-0.780462
94	17	0	3.312762	-0.345437	-1.441492

R-^{1}IM1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.228682	1.374433	1.390001
2	45	0	-0.371098	-0.088574	-0.364508
3	8	0	-2.456350	-0.178641	1.995146
4	6	0	-2.421919	-1.307083	1.364649
5	8	0	-1.659467	-1.537814	0.331119
6	8	0	-2.679656	2.024080	0.094201
7	6	0	-2.719462	1.563523	-1.114109
8	8	0	-1.871088	0.689528	-1.577069
9	8	0	0.869902	1.486883	-0.935127
10	6	0	0.798532	2.631584	-0.324058
11	8	0	0.021660	2.868144	0.688480
12	8	0	0.240799	0.668074	2.661010
13	6	0	1.060357	-0.236725	2.220575
14	8	0	1.028357	-0.706065	1.011999
15	6	0	-3.287466	-2.466867	1.821219
16	6	0	-4.115457	-2.972929	0.594917
17	1	0	-3.409205	-3.377852	-0.139210
18	1	0	-4.733523	-3.804494	0.957218
19	6	0	-4.971135	-1.911284	-0.043655

20	6	0	-4.442145	-1.108873	-1.065567
21	6	0	-6.284018	-1.669499	0.388428
22	6	0	-5.176458	-0.054188	-1.627230
23	1	0	-3.440477	-1.314797	-1.436360
24	6	0	-7.038276	-0.641441	-0.180825
25	1	0	-6.714709	-2.296173	1.165893
26	6	0	-6.485911	0.168776	-1.174845
27	1	0	-8.057832	-0.470826	0.151313
28	1	0	-7.073658	0.972581	-1.612081
29	6	0	-3.785588	2.065924	-2.069779
30	6	0	-4.539505	0.833356	-2.664045
31	1	0	-5.297435	1.232753	-3.350220
32	1	0	-3.821732	0.257802	-3.259524
33	6	0	2.117715	-0.788842	3.159390
34	6	0	1.679310	3.766488	-0.819146
35	6	0	-4.198735	-2.037239	2.970886
36	1	0	-4.817915	-2.887381	3.278366
37	1	0	-3.612662	-1.705964	3.832303
38	1	0	-4.855179	-1.213689	2.678834
39	6	0	-2.346111	-3.601655	2.272664
40	1	0	-1.753030	-3.295363	3.141146
41	1	0	-2.942513	-4.473773	2.560656
42	1	0	-1.664509	-3.886887	1.466745
43	6	0	-3.075162	2.807752	-3.219495
44	1	0	-3.820710	3.151721	-3.944001
45	1	0	-2.537424	3.685531	-2.844566
46	1	0	-2.364288	2.151358	-3.729079
47	6	0	-4.751450	3.006820	-1.347464
48	1	0	-4.224552	3.874229	-0.941240
49	1	0	-5.508757	3.360160	-2.056325
50	1	0	-5.256570	2.504549	-0.518504
51	6	0	3.009490	0.402549	3.635505
52	1	0	2.387476	1.055444	4.258895
53	1	0	3.786542	-0.028914	4.279551
54	6	0	1.405392	-1.390781	4.384690
55	1	0	0.762050	-0.650671	4.868094
56	1	0	0.794681	-2.252682	4.096435
57	1	0	2.154567	-1.733509	5.106210
58	6	0	2.630689	4.182586	0.350703
59	1	0	3.283627	4.971558	-0.044587
60	1	0	2.012520	4.627759	1.139039
61	6	0	0.770684	4.962596	-1.158338
62	1	0	0.101729	4.720936	-1.991307
63	1	0	0.163901	5.248933	-0.295358
64	1	0	1.388269	5.816083	-1.457278

65	6	0	2.480926	3.339961	-2.049437
66	1	0	3.084747	4.185211	-2.398415
67	1	0	3.147520	2.503350	-1.825582
68	1	0	1.819846	3.024543	-2.861070
69	6	0	2.956802	-1.858292	2.454967
70	1	0	3.492131	-1.443067	1.595903
71	1	0	3.690683	-2.266660	3.158948
72	1	0	2.324650	-2.673637	2.090406
73	6	0	3.626204	1.202326	2.518473
74	6	0	2.932794	2.300213	1.988276
75	6	0	4.871044	0.865141	1.965965
76	6	0	3.444115	3.050391	0.919259
77	1	0	1.974945	2.581559	2.421338
78	6	0	5.403007	1.613597	0.914228
79	1	0	5.424608	0.018249	2.365108
80	6	0	4.694647	2.696909	0.389972
81	1	0	6.369581	1.347776	0.497273
82	1	0	5.113528	3.276216	-0.429328
83	8	0	-0.422861	-3.351974	-2.421219
84	16	0	0.578706	-2.755608	-1.549188
85	8	0	0.772851	-3.251095	-0.193115
86	7	0	0.401096	-1.135367	-1.759134
87	6	0	3.195614	-3.118197	-1.582909
88	1	0	2.963524	-3.214819	-0.515602
89	8	0	2.019865	-3.009577	-2.356951
90	1	0	3.731428	-4.012850	-1.920212
91	6	0	4.117759	-1.913118	-1.780700
92	17	0	4.652905	-1.806566	-3.476670
93	17	0	5.548247	-2.205844	-0.720359
94	17	0	3.305166	-0.417231	-1.304901

R-^{3}TS1$_B$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.617298	-2.291018	-0.719395
2	45	0	-0.461629	-0.364424	0.201741
3	8	0	-2.827808	-1.009925	-1.778832
4	6	0	-2.653985	0.268313	-1.679175
5	8	0	-1.738530	0.824846	-0.934717
6	8	0	-2.933197	-2.253298	0.858579
7	6	0	-2.767893	-1.359711	1.782044
8	8	0	-1.824464	-0.462998	1.761299
9	8	0	0.778809	-1.687076	1.223670
10	6	0	0.579084	-2.967022	1.120876

11	8	0	-0.358451	-3.501171	0.400840
12	8	0	-0.266398	-2.277507	-2.278288
13	6	0	0.687143	-1.398424	-2.314448
14	8	0	0.844953	-0.468720	-1.420267
15	6	0	-3.549202	1.194732	-2.484608
16	6	0	-4.254995	2.179567	-1.498280
17	1	0	-3.482987	2.814331	-1.046101
18	1	0	-4.900213	2.825388	-2.108118
19	6	0	-5.052065	1.499738	-0.415814
20	6	0	-4.421177	1.138765	0.782597
21	6	0	-6.410816	1.192387	-0.581236
22	6	0	-5.111365	0.468477	1.802234
23	1	0	-3.378935	1.403376	0.938676
24	6	0	-7.114236	0.535184	0.431055
25	1	0	-6.918589	1.479989	-1.499274
26	6	0	-6.469077	0.170615	1.615255
27	1	0	-8.168731	0.312001	0.298922
28	1	0	-7.020973	-0.335219	2.404173
29	6	0	-3.700771	-1.337696	2.979785
30	6	0	-4.369492	0.072659	3.051749
31	1	0	-5.045029	0.054867	3.916941
32	1	0	-3.580429	0.805895	3.256350
33	6	0	1.644570	-1.456543	-3.493338
34	6	0	1.477514	-3.902479	1.914637
35	6	0	-4.580793	0.390568	-3.276854
36	1	0	-5.215906	1.078934	-3.846002
37	1	0	-4.092724	-0.292209	-3.977309
38	1	0	-5.213884	-0.205763	-2.615110
39	6	0	-2.653475	2.007973	-3.437438
40	1	0	-2.156861	1.355472	-4.164617
41	1	0	-3.264439	2.729943	-3.990284
42	1	0	-1.884677	2.554344	-2.883740
43	6	0	-2.849149	-1.537637	4.248429
44	1	0	-3.493287	-1.479532	5.132291
45	1	0	-2.366121	-2.521379	4.245280
46	1	0	-2.076478	-0.767698	4.323556
47	6	0	-4.751432	-2.441924	2.862158
48	1	0	-4.281221	-3.428691	2.827464
49	1	0	-5.416084	-2.403449	3.732626
50	1	0	-5.351799	-2.328510	1.956135
51	6	0	2.154480	-2.924549	-3.644015
52	1	0	1.286317	-3.561083	-3.846864
53	1	0	2.798054	-2.944196	-4.532785
54	6	0	0.840938	-1.074405	-4.752454
55	1	0	-0.006521	-1.751096	-4.895393

56	1	0	0.462678	-0.048521	-4.673157
57	1	0	1.490623	-1.129762	-5.632405
58	6	0	2.047028	-4.985475	0.945664
59	1	0	2.664431	-5.658310	1.554538
60	1	0	1.200533	-5.566798	0.563343
61	6	0	0.599463	-4.604230	2.970134
62	1	0	0.181003	-3.878614	3.676189
63	1	0	-0.223878	-5.145361	2.495469
64	1	0	1.209141	-5.315955	3.537245
65	6	0	2.605304	-3.126543	2.597764
66	1	0	3.256235	-3.824485	3.136922
67	1	0	3.211679	-2.576506	1.871649
68	1	0	2.204752	-2.402792	3.313226
69	6	0	2.817289	-0.495116	-3.300831
70	1	0	3.349552	-0.695052	-2.367226
71	1	0	3.523429	-0.606005	-4.132381
72	1	0	2.479842	0.544795	-3.278981
73	6	0	2.902354	-3.433971	-2.439324
74	6	0	2.201010	-4.019985	-1.375599
75	6	0	4.294653	-3.297034	-2.329178
76	6	0	2.849542	-4.429290	-0.200844
77	1	0	1.127461	-4.159599	-1.463983
78	6	0	4.959241	-3.723052	-1.176796
79	1	0	4.855991	-2.855590	-3.149915
80	6	0	4.241583	-4.276921	-0.114274
81	1	0	6.037743	-3.614661	-1.103090
82	1	0	4.761431	-4.598869	0.785470
83	8	0	0.517455	2.691632	3.065892
84	16	0	-0.114558	2.472607	1.778147
85	8	0	-1.560176	2.542829	1.619575
86	7	0	0.498938	1.159478	1.052376
87	6	0	-0.206390	4.125815	-0.275904
88	1	0	-1.020644	3.426150	-0.507639
89	8	0	0.521239	3.733324	0.867040
90	1	0	-0.625058	5.126606	-0.109316
91	6	0	0.722466	4.190109	-1.483721
92	17	0	2.110939	5.262800	-1.150678
93	17	0	-0.230612	4.872637	-2.845268
94	17	0	1.288227	2.557786	-1.892683
95	1	0	3.338986	1.364671	4.282688
96	6	0	3.590364	2.224318	3.661481
97	6	0	3.499987	2.096138	2.262228
98	6	0	3.978064	3.419740	4.244900
99	6	0	3.793316	3.224121	1.469695
100	6	0	4.271750	4.523901	3.443541

101	1	0	4.045310	3.499245	5.328202
102	6	0	4.173123	4.421355	2.054575
103	1	0	3.688012	3.157468	0.386147
104	1	0	4.567398	5.466807	3.900450
105	1	0	4.388825	5.285741	1.428849
106	6	0	3.060192	0.841505	1.660327
107	6	0	3.658098	0.416884	0.338149
108	1	0	1.817092	1.011023	1.384844
109	1	0	3.378802	1.130903	-0.451478
110	1	0	3.212565	-0.543845	0.036597
111	6	0	5.192337	0.297305	0.378944
112	6	0	5.746704	0.024015	-1.010684
113	1	0	5.398641	-0.948331	-1.386396
114	1	0	5.431677	0.791298	-1.730228
115	1	0	6.844000	0.000203	-1.003347
116	1	0	2.970429	0.023733	2.387531
117	1	0	5.580196	1.271714	0.719851
118	6	0	5.648219	-0.766083	1.368514
119	1	0	5.297913	-0.557211	2.387910
120	1	0	5.264266	-1.755120	1.077500
121	1	0	6.742659	-0.834778	1.402412

A-^{1}TS1$_{B}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.668734	-2.294040	-0.724174
2	45	0	-0.468627	-0.373800	0.161218
3	8	0	-2.902224	-1.042750	-1.777236
4	6	0	-2.713957	0.235379	-1.693453
5	8	0	-1.784429	0.785498	-0.966845
6	8	0	-2.921091	-2.200263	0.918632
7	6	0	-2.707698	-1.310267	1.833823
8	8	0	-1.751717	-0.424336	1.788407
9	8	0	0.770016	-1.684149	1.159536
10	6	0	0.564073	-2.966617	1.078392
11	8	0	-0.389887	-3.492559	0.378634
12	8	0	-0.351040	-2.290926	-2.329119
13	6	0	0.591989	-1.400828	-2.394413
14	8	0	0.787635	-0.470527	-1.510406
15	6	0	-3.612222	1.166694	-2.489036
16	6	0	-4.299262	2.153776	-1.491518
17	1	0	-3.518845	2.794617	-1.063874
18	1	0	-4.963285	2.792218	-2.088995
19	6	0	-5.063781	1.478894	-0.382641

20	6	0	-4.404154	1.153794	0.810741
21	6	0	-6.419738	1.144632	-0.516136
22	6	0	-5.063562	0.494394	1.857569
23	1	0	-3.362257	1.436062	0.937676
24	6	0	-7.092341	0.496550	0.522597
25	1	0	-6.949842	1.405454	-1.429520
26	6	0	-6.419352	0.169700	1.702209
27	1	0	-8.144963	0.252090	0.415088
28	1	0	-6.948279	-0.328088	2.511698
29	6	0	-3.609745	-1.266866	3.055527
30	6	0	-4.293874	0.138098	3.102159
31	1	0	-4.953205	0.135748	3.980045
32	1	0	-3.508791	0.883945	3.273651
33	6	0	1.510322	-1.456657	-3.606177
34	6	0	1.473794	-3.898143	1.859955
35	6	0	-4.657119	0.366623	-3.267695
36	1	0	-5.297360	1.056995	-3.828641
37	1	0	-4.180671	-0.318252	-3.974200
38	1	0	-5.282591	-0.228104	-2.597283
39	6	0	-2.727313	1.978666	-3.454020
40	1	0	-2.241523	1.324406	-4.186734
41	1	0	-3.346397	2.698330	-4.000666
42	1	0	-1.951607	2.525736	-2.910724
43	6	0	-2.728756	-1.417999	4.309661
44	1	0	-3.352467	-1.336003	5.206357
45	1	0	-2.237183	-2.397465	4.327429
46	1	0	-1.961171	-0.639889	4.340612
47	6	0	-4.651825	-2.383999	2.995747
48	1	0	-4.172091	-3.366853	2.977261
49	1	0	-5.295131	-2.327651	3.881339
50	1	0	-5.274809	-2.303273	2.101723
51	6	0	2.070855	-2.908762	-3.727815
52	1	0	1.222181	-3.577550	-3.908616
53	1	0	2.708766	-2.928658	-4.620764
54	6	0	0.653785	-1.152172	-4.850853
55	1	0	-0.171818	-1.863992	-4.939526
56	1	0	0.238364	-0.139344	-4.798080
57	1	0	1.275732	-1.217315	-5.750196
58	6	0	2.058031	-4.954552	0.870167
59	1	0	2.697387	-5.621862	1.462219
60	1	0	1.220628	-5.549501	0.488563
61	6	0	0.609328	-4.628343	2.906442
62	1	0	0.187873	-3.920813	3.628915
63	1	0	-0.212066	-5.167097	2.426058
64	1	0	1.228753	-5.345479	3.455783

65	6	0	2.594346	-3.117638	2.549148
66	1	0	3.241196	-3.812002	3.097593
67	1	0	3.207623	-2.575054	1.822491
68	1	0	2.187300	-2.390193	3.258084
69	6	0	2.648229	-0.442548	-3.485188
70	1	0	3.248933	-0.619387	-2.588461
71	1	0	3.301790	-0.517813	-4.362260
72	1	0	2.259956	0.578169	-3.430945
73	6	0	2.841198	-3.371730	-2.518920
74	6	0	2.164730	-3.971599	-1.446543
75	6	0	4.229501	-3.193893	-2.419222
76	6	0	2.833684	-4.362714	-0.277381
77	1	0	1.094903	-4.142572	-1.527663
78	6	0	4.914020	-3.595561	-1.269819
79	1	0	4.772516	-2.742743	-3.246959
80	6	0	4.221056	-4.168118	-0.200842
81	1	0	5.989740	-3.456699	-1.204444
82	1	0	4.757922	-4.476678	0.693735
83	8	0	0.572823	2.391579	2.975399
84	16	0	-0.043017	2.391636	1.660518
85	8	0	-1.484829	2.526972	1.494897
86	7	0	0.566813	1.239215	0.666907
87	6	0	-0.069893	4.293646	-0.153196
88	1	0	-0.893011	3.638369	-0.466598
89	8	0	0.612491	3.783864	0.970003
90	1	0	-0.480622	5.280187	0.097224
91	6	0	0.875007	4.473003	-1.339755
92	17	0	2.246490	5.528074	-0.895550
93	17	0	-0.089611	5.267517	-2.635509
94	17	0	1.482027	2.910143	-1.921908
95	1	0	3.303418	0.723767	4.220719
96	6	0	3.538127	1.667695	3.727905
97	6	0	3.434284	1.742656	2.327130
98	6	0	3.920339	2.772120	4.472437
99	6	0	3.708482	2.971981	1.696345
100	6	0	4.185153	3.982952	3.831624
101	1	0	4.000313	2.698815	5.555122
102	6	0	4.076315	4.079537	2.442355
103	1	0	3.592761	3.055151	0.615033
104	1	0	4.466932	4.856976	4.415929
105	1	0	4.267752	5.028702	1.945471
106	6	0	2.985998	0.580794	1.558634
107	6	0	3.630255	0.296544	0.216483
108	1	0	1.842701	0.841350	1.233348
109	1	0	3.314092	1.055266	-0.515783

110	1	0	3.246060	-0.663947	-0.164253
111	6	0	5.167377	0.258364	0.267885
112	6	0	5.730933	0.081183	-1.133942
113	1	0	5.408741	-0.876757	-1.564495
114	1	0	5.391672	0.878815	-1.807871
115	1	0	6.828399	0.089811	-1.127124
116	1	0	2.860847	-0.310874	2.183491
117	1	0	5.504546	1.233559	0.656268
118	6	0	5.670432	-0.826390	1.210215
119	1	0	5.325952	-0.666395	2.240690
120	1	0	5.313469	-1.814856	0.886536
121	1	0	6.766891	-0.859658	1.230625

R-^{3}IM2$_B$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.736232	-2.073232	-1.042796
2	45	0	-0.543322	-0.304742	0.092035
3	8	0	-2.871476	-0.636420	-1.989309
4	6	0	-2.634177	0.619038	-1.764052
5	8	0	-1.725280	1.050308	-0.938064
6	8	0	-3.074422	-2.153398	0.507124
7	6	0	-2.902091	-1.375579	1.528896
8	8	0	-1.935529	-0.508936	1.615333
9	8	0	0.634054	-1.746855	0.997532
10	6	0	0.395678	-3.003419	0.769164
11	8	0	-0.532672	-3.432487	-0.032134
12	8	0	-0.384085	-1.936353	-2.580632
13	6	0	0.564051	-1.049693	-2.543890
14	8	0	0.759992	-0.253173	-1.535877
15	6	0	-3.448506	1.675507	-2.488608
16	6	0	-4.220383	2.510521	-1.415390
17	1	0	-3.477546	3.080542	-0.844514
18	1	0	-4.839503	3.229707	-1.967632
19	6	0	-5.061614	1.694813	-0.470251
20	6	0	-4.491983	1.222832	0.720657
21	6	0	-6.400292	1.381447	-0.749100
22	6	0	-5.224879	0.440398	1.623814
23	1	0	-3.464783	1.488044	0.960677
24	6	0	-7.145862	0.612138	0.147061
25	1	0	-6.860542	1.755060	-1.661060
26	6	0	-6.562917	0.140929	1.325950
27	1	0	-8.185341	0.385593	-0.069742

28	1	0	-7.149711	-0.449933	2.025649
29	6	0	-3.859313	-1.461972	2.702732
30	6	0	-4.550200	-0.069337	2.869657
31	1	0	-5.272217	-0.176361	3.689640
32	1	0	-3.783828	0.646087	3.191630
33	6	0	1.472873	-0.959348	-3.757064
34	6	0	1.250528	-4.040729	1.476563
35	6	0	-4.415218	1.025156	-3.478179
36	1	0	-4.987119	1.805900	-3.992162
37	1	0	-3.874495	0.439856	-4.227728
38	1	0	-5.112576	0.352704	-2.972451
39	6	0	-2.475642	2.620780	-3.218852
40	1	0	-1.906136	2.088459	-3.988862
41	1	0	-3.042738	3.418765	-3.709871
42	1	0	-1.769160	3.071444	-2.515769
43	6	0	-3.037178	-1.752332	3.972670
44	1	0	-3.704830	-1.775271	4.840329
45	1	0	-2.538528	-2.725603	3.903273
46	1	0	-2.278257	-0.981062	4.130904
47	6	0	-4.893907	-2.563229	2.467676
48	1	0	-4.412548	-3.540177	2.367879
49	1	0	-5.581296	-2.600282	3.320127
50	1	0	-5.470714	-2.382771	1.557275
51	6	0	2.180434	-2.342823	-3.937262
52	1	0	1.414521	-3.067480	-4.237654
53	1	0	2.876590	-2.229692	-4.778219
54	6	0	0.592784	-0.698725	-4.994206
55	1	0	-0.159425	-1.482654	-5.113457
56	1	0	0.081053	0.266329	-4.912474
57	1	0	1.222733	-0.671609	-5.889594
58	6	0	1.990726	-4.883471	0.388311
59	1	0	2.632356	-5.591970	0.927929
60	1	0	1.235220	-5.467731	-0.150000
61	6	0	0.314049	-4.977669	2.261939
62	1	0	-0.204384	-4.434837	3.059521
63	1	0	-0.433212	-5.423998	1.600717
64	1	0	0.902344	-5.777428	2.724256
65	6	0	2.249259	-3.370269	2.419268
66	1	0	2.848598	-4.138490	2.921744
67	1	0	2.916962	-2.695697	1.877082
68	1	0	1.737257	-2.773857	3.180214
69	6	0	2.496291	0.160053	-3.590107
70	1	0	3.097566	0.019849	-2.689976
71	1	0	3.163537	0.181658	-4.459210
72	1	0	2.008596	1.136615	-3.509677

73	6	0	2.899037	-2.848051	-2.713417
74	6	0	2.195054	-3.610894	-1.769663
75	6	0	4.254192	-2.572866	-2.476023
76	6	0	2.800367	-4.079802	-0.595432
77	1	0	1.153459	-3.858293	-1.961637
78	6	0	4.876888	-3.044588	-1.316667
79	1	0	4.821413	-1.993297	-3.202113
80	6	0	4.155255	-3.785807	-0.378443
81	1	0	5.928757	-2.835091	-1.144427
82	1	0	4.647041	-4.155266	0.518868
83	8	0	0.021890	2.038036	3.561086
84	16	0	-0.222360	2.208825	2.142620
85	8	0	-1.543371	2.506736	1.620935
86	7	0	0.460939	1.029233	1.258501
87	6	0	0.338132	4.395334	0.736035
88	1	0	-0.664905	4.139040	0.370394
89	8	0	0.747181	3.539268	1.775925
90	1	0	0.327020	5.418173	1.132279
91	6	0	1.311162	4.369063	-0.443670
92	17	0	2.976601	4.687562	0.124252
93	17	0	0.791306	5.681788	-1.555928
94	17	0	1.257763	2.810574	-1.287105
95	1	0	4.450636	-1.437415	3.652268
96	6	0	4.097838	-0.406043	3.699691
97	6	0	3.891320	0.295674	2.480206
98	6	0	3.863874	0.196112	4.921826
99	6	0	3.433521	1.640087	2.572446
100	6	0	3.413466	1.519599	4.985285
101	1	0	4.030737	-0.364491	5.840786
102	6	0	3.201005	2.232300	3.802792
103	1	0	3.257683	2.211985	1.660752
104	1	0	3.222048	1.987675	5.948754
105	1	0	2.833431	3.256155	3.839657
106	6	0	4.137550	-0.334316	1.239087
107	6	0	4.022803	0.329759	-0.085304
108	1	0	1.291076	0.661755	1.738272
109	1	0	3.105446	0.938396	-0.143922
110	1	0	3.920215	-0.444172	-0.860428
111	6	0	5.233067	1.228610	-0.427756
112	6	0	5.045595	1.912809	-1.773195
113	1	0	5.079837	1.177673	-2.590335
114	1	0	4.083141	2.436571	-1.837212
115	1	0	5.840478	2.645614	-1.961404
116	1	0	4.527983	-1.354708	1.265363
117	1	0	5.289221	2.004865	0.354212

118	6	0	6.533591	0.437035	-0.406068
119	1	0	6.704194	-0.042077	0.565922
120	1	0	6.512783	-0.354556	-1.170046
121	1	0	7.396894	1.078012	-0.622766

R-^{3}TS2$_B$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.054136	-2.636551	1.023954
2	45	0	-0.105562	-0.507499	-0.118189
3	8	0	1.714565	-1.963371	2.019291
4	6	0	2.221058	-0.799037	1.753766
5	8	0	1.718787	0.039732	0.898526
6	8	0	1.247449	-3.456247	-0.415425
7	6	0	1.453492	-2.808026	-1.530589
8	8	0	0.975892	-1.637036	-1.760043
9	8	0	-1.892583	-1.219869	-1.051309
10	6	0	-2.204932	-2.466472	-0.887078
11	8	0	-1.604547	-3.270224	-0.062392
12	8	0	-1.127918	-1.940521	2.568429
13	6	0	-1.523363	-0.700280	2.589362
14	8	0	-1.245451	0.136183	1.651450
15	6	0	3.487039	-0.393499	2.498760
16	6	0	4.598565	-0.072753	1.450114
17	1	0	4.291968	0.813463	0.884496
18	1	0	5.496034	0.204162	2.019191
19	6	0	4.910031	-1.198164	0.498595
20	6	0	4.166969	-1.356106	-0.681420
21	6	0	5.939164	-2.111030	0.773888
22	6	0	4.425242	-2.407349	-1.573143
23	1	0	3.375834	-0.646556	-0.920300
24	6	0	6.216009	-3.155049	-0.110521
25	1	0	6.529688	-1.990989	1.679464
26	6	0	5.463583	-3.303270	-1.276625
27	1	0	7.022574	-3.849016	0.106253
28	1	0	5.682275	-4.113075	-1.968757
29	6	0	2.311349	-3.468386	-2.600049
30	6	0	3.578299	-2.574262	-2.805472
31	1	0	4.161767	-3.038726	-3.611473
32	1	0	3.235733	-1.594553	-3.160206
33	6	0	-2.375132	-0.254975	3.767304
34	6	0	-3.376047	-3.045763	-1.671512
35	6	0	-3.696340	-1.089331	3.749343

36	1	0	-3.439753	-2.117330	4.029188
37	1	0	-4.338288	-0.681185	4.541346
38	6	0	-4.521668	-3.352174	-0.649239
39	1	0	-5.404147	-3.639020	-1.236114
40	1	0	-4.214966	-4.226308	-0.063392
41	6	0	-4.422457	-1.100978	2.429246
42	6	0	-4.192038	-2.147657	1.526141
43	6	0	-5.325997	-0.089015	2.064569
44	6	0	-4.840875	-2.214308	0.284380
45	1	0	-3.488424	-2.932136	1.796961
46	6	0	-5.983628	-0.140019	0.833220
47	1	0	-5.531928	0.723078	2.758036
48	6	0	-5.748420	-1.197407	-0.050904
49	1	0	-6.690610	0.640336	0.564882
50	1	0	-6.282249	-1.244495	-0.997969
51	8	0	0.222843	3.147877	-2.767800
52	16	0	0.841634	2.065213	-2.010911
53	8	0	1.996170	1.378263	-2.570897
54	7	0	-0.333001	1.091690	-1.421146
55	6	0	2.655235	2.715494	-0.207957
56	1	0	2.771831	2.211282	0.754855
57	8	0	1.288164	2.669381	-0.535779
58	1	0	3.270403	2.208007	-0.960504
59	6	0	3.116917	4.160553	-0.074290
60	17	0	2.972198	5.008372	-1.629654
61	17	0	4.825396	4.112444	0.458234
62	17	0	2.133452	5.004088	1.162184
63	6	0	-2.182602	2.420270	-0.439197
64	1	0	-0.930889	0.812281	-2.205065
65	1	0	-2.308928	1.548687	0.208799
66	6	0	-2.995120	2.475104	-1.601240
67	6	0	-2.904823	3.530852	-2.541833
68	6	0	-3.951385	1.454293	-1.812055
69	6	0	-3.753692	3.564410	-3.633320
70	1	0	-2.136771	4.291231	-2.420502
71	6	0	-4.810235	1.509170	-2.896818
72	1	0	-4.001924	0.634281	-1.095142
73	6	0	-4.713585	2.562403	-3.809543
74	1	0	-3.670157	4.369644	-4.360040
75	1	0	-5.554390	0.727257	-3.042197
76	1	0	-5.381593	2.598542	-4.668306
77	6	0	-1.481555	3.595156	0.115707
78	1	0	-0.845466	3.289245	0.956347
79	1	0	-0.819707	4.045559	-0.637941
80	6	0	-2.474242	4.696246	0.580681

81	6	0	-1.693663	5.889416	1.108648
82	6	0	-3.466268	4.186956	1.615805
83	1	0	-3.040747	5.011831	-0.310384
84	1	0	-0.989589	6.278861	0.363711
85	1	0	-2.369230	6.704305	1.396238
86	1	0	-1.112685	5.612692	1.998788
87	1	0	-4.059986	3.340621	1.241859
88	1	0	-2.947239	3.853614	2.523846
89	1	0	-4.165310	4.979674	1.908065
90	6	0	1.518590	-3.475954	-3.918639
91	1	0	2.142609	-3.884525	-4.721203
92	1	0	0.624259	-4.102664	-3.833509
93	1	0	1.211443	-2.462087	-4.188882
94	6	0	2.697057	-4.891952	-2.200723
95	1	0	1.806267	-5.513382	-2.069098
96	1	0	3.319129	-5.338236	-2.985859
97	1	0	3.252480	-4.907813	-1.260060
98	6	0	3.190935	0.879009	3.314574
99	1	0	2.430962	0.683314	4.079361
100	1	0	4.103902	1.214380	3.818595
101	1	0	2.828950	1.693472	2.678693
102	6	0	3.948297	-1.512760	3.434884
103	1	0	4.867281	-1.203123	3.946214
104	1	0	3.187008	-1.731989	4.188228
105	1	0	4.145127	-2.436014	2.884810
106	6	0	-2.934830	-4.365163	-2.325033
107	1	0	-3.789599	-4.833164	-2.825967
108	1	0	-2.158133	-4.185937	-3.076108
109	1	0	-2.538353	-5.056169	-1.577553
110	6	0	-3.860488	-2.066287	-2.739147
111	1	0	-3.051038	-1.793385	-3.423019
112	1	0	-4.667818	-2.527814	-3.319562
113	1	0	-4.234320	-1.144820	-2.289583
114	6	0	-2.676686	1.239414	3.660800
115	1	0	-3.293381	1.557889	4.509332
116	1	0	-1.751295	1.824016	3.662762
117	1	0	-3.209462	1.467869	2.733623
118	6	0	-1.623839	-0.561858	5.073240
119	1	0	-0.701446	0.025099	5.140783
120	1	0	-2.253936	-0.304856	5.931824
121	1	0	-1.362983	-1.621734	5.129856

R-^{1}PC$_B$

Center	Atomic	Atomic	Coordinates (Angstroms)

RSC Advances

Number	Number	Type	X	Y	Z
1	45	0	-0.693768	-2.155649	-1.627438
2	45	0	-0.152768	-0.465515	0.014182
3	8	0	-2.333038	-1.058632	-2.183386
4	6	0	-2.583947	0.071394	-1.604670
5	8	0	-1.833192	0.606297	-0.683374
6	8	0	-1.832722	-3.102672	-0.163185
7	6	0	-1.884909	-2.613734	1.030896
8	8	0	-1.276584	-1.517946	1.397866
9	8	0	1.477313	-1.645294	0.581336
10	6	0	1.700683	-2.772653	-0.030402
11	8	0	0.957952	-3.235429	-0.983876
12	8	0	0.476850	-1.095859	-2.976113
13	6	0	1.109518	-0.027172	-2.594664
14	8	0	1.036031	0.482397	-1.403033
15	6	0	-3.833567	0.826642	-2.044049
16	6	0	-4.696032	1.151163	-0.784940
17	1	0	-4.104734	1.803922	-0.129850
18	1	0	-5.562412	1.728004	-1.134463
19	6	0	-5.143852	-0.063387	-0.014396
20	6	0	-4.313388	-0.599007	0.979687
21	6	0	-6.365483	-0.698642	-0.286060
22	6	0	-4.668355	-1.757357	1.685256
23	1	0	-3.379562	-0.098858	1.222005
24	6	0	-6.739081	-1.844300	0.419998
25	1	0	-7.025653	-0.287689	-1.046621
26	6	0	-5.894033	-2.374802	1.396695
27	1	0	-7.691352	-2.322130	0.210150
28	1	0	-6.185964	-3.267195	1.945587
29	6	0	-2.684523	-3.338176	2.102379
30	6	0	-3.718028	-2.332654	2.701458
31	1	0	-4.268603	-2.871295	3.483945
32	1	0	-3.155875	-1.524027	3.183609
33	6	0	1.970934	0.676412	-3.635784
34	6	0	2.889367	-3.619777	0.401577
35	6	0	-4.636837	-0.006171	-3.046522
36	1	0	-5.526168	0.555935	-3.354617
37	1	0	-4.039671	-0.231006	-3.933676
38	1	0	-4.955610	-0.956308	-2.611084
39	6	0	-3.399853	2.148184	-2.703566
40	1	0	-2.777679	1.961735	-3.586241
41	1	0	-4.285117	2.709414	-3.021817
42	1	0	-2.823822	2.771059	-2.013941
43	6	0	-1.713063	-3.762176	3.220812
44	1	0	-2.272497	-4.251394	4.025507

45	1	0	-0.969510	-4.473311	2.844534
46	1	0	-1.190538	-2.894542	3.635538
47	6	0	-3.382244	-4.566908	1.518083
48	1	0	-2.653034	-5.279428	1.123290
49	1	0	-3.965496	-5.063202	2.302245
50	1	0	-4.054307	-4.294290	0.700943
51	6	0	2.935499	-0.370213	-4.274927
52	1	0	2.320345	-1.129553	-4.770491
53	1	0	3.507068	0.156950	-5.049987
54	6	0	1.029223	1.210764	-4.732460
55	1	0	0.448202	0.397023	-5.175717
56	1	0	0.332865	1.952153	-4.323876
57	1	0	1.617595	1.695882	-5.518876
58	6	0	3.738106	-3.969778	-0.861078
59	1	0	4.572065	-4.594966	-0.516547
60	1	0	3.112653	-4.582653	-1.519761
61	6	0	2.336626	-4.930075	0.995231
62	1	0	1.761494	-4.732864	1.906588
63	1	0	1.688676	-5.439521	0.276267
64	1	0	3.167185	-5.594795	1.256953
65	6	0	3.744493	-2.889258	1.435970
66	1	0	4.581084	-3.529306	1.739193
67	1	0	4.150632	-1.959114	1.028411
68	1	0	3.161623	-2.640427	2.327474
69	6	0	2.764573	1.824748	-3.011738
70	1	0	3.452433	1.462748	-2.241053
71	1	0	3.351760	2.328637	-3.788611
72	1	0	2.103200	2.558508	-2.543797
73	6	0	3.864775	-1.024023	-3.286787
74	6	0	3.448618	-2.167851	-2.591351
75	6	0	5.136361	-0.497514	-3.011788
76	6	0	4.253699	-2.771812	-1.614776
77	1	0	2.478404	-2.600528	-2.819672
78	6	0	5.959381	-1.099071	-2.057699
79	1	0	5.479847	0.380664	-3.553668
80	6	0	5.519295	-2.223611	-1.355412
81	1	0	6.945652	-0.689878	-1.859386
82	1	0	6.162193	-2.687906	-0.610891
83	8	0	-0.156820	2.982323	3.252444
84	16	0	-0.682430	2.058699	2.265650
85	8	0	-2.017966	1.514450	2.396465
86	7	0	0.368113	0.759778	1.932414
87	6	0	-1.515966	3.668771	0.440429
88	1	0	-2.318473	3.137655	-0.086356
89	8	0	-0.503273	2.740288	0.793936

90	1	0	-1.921696	4.194827	1.314397
91	6	0	-0.882730	4.699869	-0.480802
92	17	0	0.382985	5.600634	0.395249
93	17	0	-2.190342	5.806034	-0.991665
94	17	0	-0.168071	3.904451	-1.902223
95	1	0	2.004264	-1.233237	3.622808
96	6	0	2.241327	-0.348124	4.218983
97	6	0	2.226297	0.906340	3.598161
98	6	0	2.549888	-0.475142	5.568984
99	6	0	2.536922	2.036076	4.357382
100	6	0	2.859556	0.658985	6.315873
101	1	0	2.557532	-1.458656	6.036024
102	6	0	2.853302	1.911475	5.707244
103	1	0	2.513444	3.021125	3.894312
104	1	0	3.106433	0.566634	7.372105
105	1	0	3.092356	2.800013	6.288619
106	6	0	1.857817	0.961293	2.134466
107	6	0	2.347907	2.149935	1.326453
108	1	0	0.030156	0.002254	2.538438
109	1	0	1.962014	3.090624	1.743707
110	1	0	1.922410	2.056077	0.316030
111	6	0	3.870689	2.228558	1.200992
112	6	0	4.233230	3.419458	0.323004
113	1	0	3.818345	3.301545	-0.687496
114	1	0	3.833287	4.356704	0.730760
115	1	0	5.319939	3.530892	0.226501
116	1	0	2.243027	0.048421	1.663415
117	1	0	4.300518	2.400940	2.201858
118	6	0	4.455278	0.928447	0.654799
119	1	0	4.457264	0.135736	1.414031
120	1	0	3.876148	0.554493	-0.204280
121	1	0	5.492925	1.063123	0.325364

R-^{3}TS1$_T$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.468949	-0.889162	1.981909
2	45	0	-0.645918	-0.444609	-0.257142
3	8	0	-3.061962	-1.908943	1.181346
4	6	0	-3.144624	-2.025860	-0.107010
5	8	0	-2.289824	-1.502936	-0.938029
6	8	0	-2.538173	0.864648	1.907390

7	6	0	-2.472876	1.616543	0.858284
8	8	0	-1.753650	1.334495	-0.192751
9	8	0	0.983050	0.515778	0.595403
10	6	0	1.063599	0.617933	1.890224
11	8	0	0.162778	0.157823	2.704771
12	8	0	-0.399378	-2.659286	1.982064
13	6	0	0.358917	-2.942537	0.967118
14	8	0	0.457656	-2.197407	-0.092080
15	6	0	-4.286101	-2.816250	-0.719271
16	6	0	-5.045018	-1.881845	-1.717006
17	1	0	-4.359551	-1.650440	-2.540013
18	1	0	-5.873305	-2.472438	-2.129098
19	6	0	-5.555474	-0.607524	-1.098458
20	6	0	-4.743223	0.536213	-1.086168
21	6	0	-6.819964	-0.539341	-0.493973
22	6	0	-5.151826	1.720488	-0.455584
23	1	0	-3.775359	0.504855	-1.583245
24	6	0	-7.251787	0.641019	0.114053
25	1	0	-7.468423	-1.411901	-0.512158
26	6	0	-6.420653	1.762764	0.141093
27	1	0	-8.238072	0.687477	0.565601
28	1	0	-6.758458	2.680502	0.616906
29	6	0	-3.265307	2.913852	0.835658
30	6	0	-4.220514	2.901691	-0.401227
31	1	0	-4.788481	3.840541	-0.365286
32	1	0	-3.599820	2.929121	-1.304336
33	6	0	1.151946	-4.238159	1.016394
34	6	0	2.251605	1.349406	2.488532
35	6	0	-5.220673	-3.343152	0.369390
36	1	0	-6.037058	-3.907963	-0.094786
37	1	0	-4.684981	-4.006481	1.053950
38	1	0	-5.646839	-2.530325	0.962757
39	6	0	-3.674940	-3.983940	-1.518534
40	1	0	-3.163856	-4.686349	-0.851503
41	1	0	-4.472111	-4.528244	-2.035945
42	1	0	-2.955745	-3.619021	-2.256986
43	6	0	-2.270439	4.077652	0.669388
44	1	0	-2.814803	5.028736	0.679960
45	1	0	-1.536826	4.094986	1.484074
46	1	0	-1.727850	3.995994	-0.279118
47	6	0	-4.060657	3.073325	2.132607
48	1	0	-3.396972	3.090704	3.000950
49	1	0	-4.620654	4.014762	2.100613
50	1	0	-4.765994	2.249579	2.269355
51	6	0	1.931975	-4.298357	2.367076

52	1	0	1.192277	-4.293361	3.176026
53	1	0	2.442624	-5.269687	2.390659
54	6	0	0.133821	-5.397037	0.984080
55	1	0	-0.574665	-5.321557	1.814014
56	1	0	-0.424283	-5.397301	0.041689
57	1	0	0.667552	-6.350280	1.061681
58	6	0	2.844778	0.487921	3.646722
59	1	0	3.651090	1.080735	4.097415
60	1	0	2.064435	0.358823	4.405338
61	6	0	1.710873	2.676027	3.064242
62	1	0	1.290613	3.303009	2.267182
63	1	0	0.938563	2.491224	3.817165
64	1	0	2.531498	3.236738	3.524586
65	6	0	3.309925	1.633073	1.423492
66	1	0	4.150537	2.170871	1.877754
67	1	0	3.687749	0.711857	0.970749
68	1	0	2.897672	2.254757	0.624162
69	6	0	2.101659	-4.342663	-0.177088
70	1	0	2.853304	-3.547142	-0.155614
71	1	0	2.621061	-5.307121	-0.146396
72	1	0	1.551645	-4.267102	-1.120167
73	6	0	2.924755	-3.181879	2.569932
74	6	0	2.490324	-1.938054	3.053168
75	6	0	4.286289	-3.347299	2.275039
76	6	0	3.369272	-0.855020	3.203803
77	1	0	1.447192	-1.815379	3.330394
78	6	0	5.182687	-2.291223	2.458120
79	1	0	4.642657	-4.307804	1.909949
80	6	0	4.726495	-1.048922	2.905542
81	1	0	6.237902	-2.434187	2.243178
82	1	0	5.425076	-0.224280	3.027265
83	8	0	-0.036414	-0.380560	-4.618546
84	16	0	0.358318	-0.973209	-3.353730
85	8	0	0.052750	-2.357854	-3.033746
86	7	0	-0.027839	0.001985	-2.109462
87	6	0	2.656439	-1.357021	-2.244228
88	1	0	2.122345	-1.079300	-1.325004
89	8	0	2.021323	-0.826321	-3.395144
90	1	0	2.716567	-2.451242	-2.302748
91	6	0	4.064362	-0.799368	-2.152562
92	17	0	5.037485	-1.279614	-3.563278
93	17	0	4.769773	-1.474343	-0.649416
94	17	0	4.029546	0.984855	-2.035159
95	6	0	0.298978	2.518896	-2.807838
96	6	0	0.842941	3.107407	-1.524303

97	1	0	0.201088	1.279365	-2.479938
98	1	0	1.811939	2.639949	-1.293121
99	1	0	0.176139	2.856051	-0.687114
100	6	0	1.029035	4.635734	-1.585034
101	1	0	0.064806	5.115054	-1.809886
102	6	0	-1.136690	2.850440	-3.126574
103	1	0	-1.242073	3.911514	-3.404651
104	1	0	-1.496985	2.254218	-3.973347
105	1	0	-1.782588	2.652475	-2.263428
106	6	0	1.223463	2.580076	-3.993989
107	1	0	1.233101	3.600113	-4.411598
108	1	0	2.254311	2.319086	-3.730259
109	1	0	0.893508	1.907610	-4.792978
110	1	0	1.701461	4.880487	-2.420732
111	6	0	1.581993	5.184334	-0.301446
112	6	0	2.912261	4.941207	0.061657
113	6	0	0.782046	5.920830	0.577551
114	6	0	3.425886	5.418098	1.263254
115	1	0	3.553754	4.370511	-0.612965
116	6	0	1.290199	6.398533	1.783529
117	1	0	-0.252428	6.130959	0.303309
118	6	0	2.615125	6.148100	2.130437
119	1	0	4.464788	5.219183	1.523395
120	1	0	0.650007	6.974413	2.450183
121	1	0	3.015504	6.522375	3.071076

R-^{1}TS1$_{T}$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-1.878754	0.081038	2.147236
2	45	0	-0.505210	-0.240810	0.175315
3	8	0	-2.864284	-1.683774	1.680127
4	6	0	-2.547740	-2.313311	0.594203
5	8	0	-1.622438	-1.922555	-0.236127
6	8	0	-3.198220	1.153482	0.984015
7	6	0	-2.934827	1.374164	-0.260190
8	8	0	-1.862056	0.925787	-0.857384
9	8	0	0.539325	1.490839	0.662057
10	6	0	0.161981	2.174539	1.701068
11	8	0	-0.819587	1.839478	2.482913
12	8	0	-0.554783	-1.012213	3.282319
13	6	0	0.496721	-1.491841	2.686457
14	8	0	0.757719	-1.317374	1.430411

15	6	0	-3.260361	-3.605088	0.235252
16	6	0	-3.786816	-3.487269	-1.231712
17	1	0	-2.916100	-3.417746	-1.893807
18	1	0	-4.302622	-4.429977	-1.455776
19	6	0	-4.701887	-2.313359	-1.458596
20	6	0	-4.167858	-1.077398	-1.852219
21	6	0	-6.085599	-2.408059	-1.244025
22	6	0	-4.975620	0.061363	-1.988555
23	1	0	-3.101425	-1.006215	-2.058591
24	6	0	-6.906834	-1.290299	-1.404831
25	1	0	-6.517236	-3.364349	-0.958052
26	6	0	-6.355165	-0.059018	-1.764458
27	1	0	-7.977709	-1.378528	-1.249046
28	1	0	-6.995215	0.812391	-1.883199
29	6	0	-3.882210	2.218064	-1.094399
30	6	0	-4.347136	1.385338	-2.332195
31	1	0	-5.052446	2.018435	-2.886586
32	1	0	-3.474749	1.225414	-2.976569
33	6	0	1.470686	-2.315520	3.511164
34	6	0	0.899078	3.466279	2.016859
35	6	0	-4.400991	-3.882938	1.214621
36	1	0	-4.892629	-4.823689	0.941494
37	1	0	-4.024126	-3.970513	2.237042
38	1	0	-5.144948	-3.082003	1.202402
39	6	0	-2.218221	-4.740782	0.286573
40	1	0	-1.832069	-4.868446	1.303928
41	1	0	-2.691332	-5.681266	-0.016482
42	1	0	-1.376901	-4.533082	-0.380591
43	6	0	-3.095825	3.443417	-1.599485
44	1	0	-3.742714	4.062495	-2.230474
45	1	0	-2.746924	4.057500	-0.761082
46	1	0	-2.225968	3.129930	-2.187711
47	6	0	-5.080076	2.661658	-0.253721
48	1	0	-4.756570	3.244233	0.612869
49	1	0	-5.744273	3.282022	-0.865664
50	1	0	-5.644451	1.802164	0.116474
51	6	0	1.921190	-1.457343	4.736055
52	1	0	1.037204	-1.279006	5.358979
53	1	0	2.616413	-2.078492	5.315678
54	6	0	0.714219	-3.554734	4.026923
55	1	0	-0.167712	-3.263450	4.604033
56	1	0	0.394765	-4.188185	3.192419
57	1	0	1.377216	-4.146317	4.667327
58	6	0	1.413207	3.389449	3.489211
59	1	0	1.935098	4.334378	3.689271

60	1	0	0.537703	3.347290	4.147164
61	6	0	-0.117168	4.618624	1.901264
62	1	0	-0.490373	4.695474	0.872666
63	1	0	-0.963337	4.465106	2.576943
64	1	0	0.372938	5.567024	2.149257
65	6	0	2.055347	3.694007	1.041639
66	1	0	2.583120	4.616078	1.312457
67	1	0	2.765876	2.863083	1.057434
68	1	0	1.687251	3.805439	0.016609
69	6	0	2.670458	-2.744130	2.663106
70	1	0	3.226629	-1.877567	2.294432
71	1	0	3.343856	-3.359189	3.270597
72	1	0	2.346476	-3.328023	1.796248
73	6	0	2.564148	-0.145895	4.367639
74	6	0	1.767087	0.991252	4.168526
75	6	0	3.950417	-0.033575	4.182960
76	6	0	2.317167	2.215454	3.762203
77	1	0	0.694898	0.922834	4.335023
78	6	0	4.517123	1.184741	3.802337
79	1	0	4.583758	-0.902419	4.346660
80	6	0	3.706533	2.301176	3.585851
81	1	0	5.592472	1.264423	3.675299
82	1	0	4.150641	3.247516	3.285806
83	8	0	-0.024402	-2.325109	-3.086435
84	16	0	0.840820	-2.155978	-1.932771
85	8	0	0.898336	-3.138180	-0.860803
86	7	0	0.832583	-0.650031	-1.240959
87	6	0	3.405763	-1.897725	-1.705076
88	1	0	3.684230	-0.835678	-1.689088
89	8	0	2.355570	-2.116805	-2.630436
90	1	0	3.119803	-2.207520	-0.692100
91	6	0	4.613003	-2.715565	-2.137400
92	17	0	4.237392	-4.451456	-2.117630
93	17	0	5.923173	-2.363559	-0.964364
94	17	0	5.128731	-2.224360	-3.774833
95	6	0	0.783894	0.994183	-3.289686
96	6	0	1.012279	2.280039	-2.521471
97	1	0	0.799420	0.206913	-2.361956
98	1	0	1.967072	2.219819	-1.977468
99	1	0	0.233393	2.399087	-1.753360
100	6	0	1.024040	3.530629	-3.423977
101	1	0	0.045525	3.630467	-3.915618
102	6	0	-0.577126	0.848727	-3.920120
103	1	0	-0.632696	1.452649	-4.839555
104	1	0	-0.775581	-0.191533	-4.202423

105	1	0	-1.363342	1.176658	-3.232827
106	6	0	1.918297	0.575046	-4.190193
107	1	0	1.983378	1.259827	-5.050154
108	1	0	2.886539	0.597853	-3.675838
109	1	0	1.767085	-0.432707	-4.590818
110	1	0	1.768753	3.397079	-4.221406
111	6	0	1.336070	4.761351	-2.626412
112	6	0	2.661252	5.159913	-2.419729
113	6	0	0.317003	5.497515	-2.013164
114	6	0	2.960295	6.265713	-1.630087
115	1	0	3.466208	4.592454	-2.888838
116	6	0	0.611548	6.603855	-1.221255
117	1	0	-0.721533	5.200607	-2.167977
118	6	0	1.935285	6.990606	-1.025731
119	1	0	3.997778	6.563740	-1.486747
120	1	0	-0.196449	7.165799	-0.754542
121	1	0	2.167856	7.856574	-0.408479

R-^{3}IM2$_T$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.409104	-0.859649	-2.035386
2	45	0	0.601439	-0.504438	0.216792
3	8	0	3.026597	-1.872414	-1.274172
4	6	0	3.134124	-2.005097	0.012151
5	8	0	2.280471	-1.512994	0.861300
6	8	0	2.438234	0.913164	-1.908563
7	6	0	2.349385	1.641628	-0.843398
8	8	0	1.634751	1.313317	0.197573
9	8	0	-1.047965	0.465257	-0.571701
10	6	0	-1.142118	0.609214	-1.860639
11	8	0	-0.249343	0.174923	-2.700322
12	8	0	0.365738	-2.643049	-2.078431
13	6	0	-0.354917	-2.988563	-1.054719
14	8	0	-0.435905	-2.287803	0.035676
15	6	0	4.299496	-2.778672	0.597685
16	6	0	5.030810	-1.851230	1.622547
17	1	0	4.338753	-1.664429	2.451318
18	1	0	5.876587	-2.428415	2.017615
19	6	0	5.502235	-0.545520	1.039637
20	6	0	4.659643	0.575746	1.062042
21	6	0	6.761146	-0.426523	0.431246
22	6	0	5.031748	1.786733	0.460287

23	1	0	3.697326	0.505535	1.565536
24	6	0	7.157077	0.780390	-0.148227
25	1	0	7.433387	-1.281106	0.423671
26	6	0	6.295378	1.878911	-0.142713
27	1	0	8.139120	0.865681	-0.603142
28	1	0	6.604900	2.817288	-0.597047
29	6	0	3.106025	2.958476	-0.791879
30	6	0	4.066016	2.940974	0.441946
31	1	0	4.605834	3.896913	0.428252
32	1	0	3.447683	2.925745	1.347413
33	6	0	-1.120909	-4.297438	-1.131091
34	6	0	-2.335254	1.352379	-2.430337
35	6	0	5.246056	-3.245618	-0.507607
36	1	0	6.081037	-3.797715	-0.061739
37	1	0	4.728628	-3.905532	-1.209378
38	1	0	5.645579	-2.403549	-1.078434
39	6	0	3.720810	-3.984807	1.363551
40	1	0	3.222426	-4.678611	0.677927
41	1	0	4.533572	-4.525204	1.860288
42	1	0	2.997461	-3.657187	2.115083
43	6	0	2.083416	4.092466	-0.592779
44	1	0	2.606164	5.055695	-0.583357
45	1	0	1.344081	4.114122	-1.402246
46	1	0	1.550340	3.974788	0.356843
47	6	0	3.891342	3.171172	-2.087418
48	1	0	3.223696	3.190143	-2.952747
49	1	0	4.423360	4.127761	-2.034602
50	1	0	4.620478	2.372700	-2.246474
51	6	0	-1.950642	-4.315359	-2.453121
52	1	0	-1.241371	-4.274510	-3.288029
53	1	0	-2.453150	-5.290338	-2.493361
54	6	0	-0.079790	-5.434739	-1.189053
55	1	0	0.593325	-5.308307	-2.041899
56	1	0	0.515707	-5.463888	-0.270399
57	1	0	-0.597370	-6.394824	-1.287832
58	6	0	-2.957853	0.492773	-3.575382
59	1	0	-3.785361	1.080254	-3.993316
60	1	0	-2.200624	0.380891	-4.359855
61	6	0	-1.795596	2.672495	-3.020761
62	1	0	-1.352622	3.296332	-2.233933
63	1	0	-1.041073	2.479014	-3.789205
64	1	0	-2.620507	3.239728	-3.464943
65	6	0	-3.367506	1.646552	-1.343151
66	1	0	-4.204227	2.206003	-1.777823
67	1	0	-3.753353	0.728700	-0.890629

68	1	0	-2.926774	2.251140	-0.545356
69	6	0	-2.020148	-4.472744	0.093580
70	1	0	-2.778282	-3.685060	0.149853
71	1	0	-2.531226	-5.440223	0.034331
72	1	0	-1.431707	-4.442613	1.015975
73	6	0	-2.959239	-3.201503	-2.580408
74	6	0	-2.556304	-1.941531	-3.049107
75	6	0	-4.304779	-3.386679	-2.228594
76	6	0	-3.449461	-0.862750	-3.132769
77	1	0	-1.527012	-1.802351	-3.367861
78	6	0	-5.215280	-2.332470	-2.338691
79	1	0	-4.638043	-4.360059	-1.875827
80	6	0	-4.789595	-1.075627	-2.775474
81	1	0	-6.258029	-2.489311	-2.077845
82	1	0	-5.499513	-0.254797	-2.846529
83	8	0	0.243565	-0.441633	4.599376
84	16	0	-0.170579	-1.108944	3.379018
85	8	0	0.318562	-2.420778	3.003815
86	7	0	-0.061288	-0.119432	2.096858
87	6	0	-2.528949	-1.770634	2.507949
88	1	0	-1.944248	-1.719061	1.579306
89	8	0	-1.820884	-1.246081	3.613716
90	1	0	-2.803443	-2.817272	2.695248
91	6	0	-3.809017	-0.968850	2.312547
92	17	0	-4.909358	-1.188373	3.698861
93	17	0	-4.582509	-1.577855	0.813506
94	17	0	-3.436844	0.763534	2.120314
95	6	0	-0.471755	2.887231	2.963766
96	6	0	-1.001145	3.365704	1.651392
97	1	0	-0.350232	0.842771	2.336191
98	1	0	-2.021963	2.984192	1.491596
99	1	0	-0.392808	2.968848	0.822334
100	6	0	-1.055651	4.906921	1.542805
101	1	0	-0.048409	5.320134	1.699356
102	6	0	1.003952	2.859333	3.173676
103	1	0	1.415721	3.874502	3.327582
104	1	0	1.275281	2.269738	4.058020
105	1	0	1.522010	2.431804	2.303554
106	6	0	-1.355663	2.890958	4.163118
107	1	0	-1.185472	3.784628	4.789667
108	1	0	-2.419012	2.879272	3.896030
109	1	0	-1.157713	2.024329	4.810075
110	1	0	-1.675828	5.288545	2.368271
111	6	0	-1.599396	5.378395	0.224349
112	6	0	-2.921951	5.099551	-0.143858

113	6	0	-0.800359	6.087568	-0.677128
114	6	0	-3.427293	5.517628	-1.370514
115	1	0	-3.565258	4.549946	0.546047
116	6	0	-1.299964	6.505374	-1.908506
117	1	0	0.228263	6.322916	-0.401195
118	6	0	-2.617038	6.221870	-2.259317
119	1	0	-4.460236	5.292770	-1.633684
120	1	0	-0.659287	7.060127	-2.592483
121	1	0	-3.011734	6.550463	-3.219313

R-^{3}TS2$_T$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.605113	-0.684414	-2.088810
2	45	0	0.606803	-0.374052	0.124440
3	8	0	3.101219	-1.793627	-1.193127
4	6	0	3.093182	-1.946892	0.094871
5	8	0	2.202747	-1.434695	0.892144
6	8	0	2.683763	1.042058	-1.807658
7	6	0	2.524822	1.759423	-0.741712
8	8	0	1.712006	1.436314	0.218478
9	8	0	-0.941296	0.688268	-0.768421
10	6	0	-0.889634	0.916776	-2.047746
11	8	0	0.039501	0.466875	-2.834719
12	8	0	0.496907	-2.413389	-2.287981
13	6	0	-0.275814	-2.809253	-1.318693
14	8	0	-0.415922	-2.155742	-0.211582
15	6	0	4.177880	-2.783068	0.749798
16	6	0	4.886003	-1.898107	1.827241
17	1	0	4.155223	-1.694157	2.617990
18	1	0	5.686395	-2.511115	2.261522
19	6	0	5.437656	-0.602114	1.293556
20	6	0	4.638117	0.551115	1.295972
21	6	0	6.730875	-0.520372	0.755076
22	6	0	5.091576	1.760157	0.748183
23	1	0	3.643442	0.505505	1.736202
24	6	0	7.204351	0.682135	0.226369
25	1	0	7.368760	-1.400798	0.762053
26	6	0	6.388234	1.814977	0.216117
27	1	0	8.211284	0.737186	-0.176025
28	1	0	6.759011	2.750532	-0.195910
29	6	0	3.309940	3.051833	-0.593948
30	6	0	4.176437	2.954865	0.703833
31	1	0	4.753093	3.887126	0.766189

32	1	0	3.492194	2.932437	1.560788
33	6	0	-1.047359	-4.104825	-1.500336
34	6	0	-1.980843	1.766694	-2.678584
35	6	0	-1.938375	-3.969580	-2.777042
36	1	0	-1.269771	-3.908868	-3.643746
37	1	0	-2.507299	-4.904627	-2.861746
38	6	0	-2.705131	0.900023	-3.760124
39	1	0	-3.514932	1.519774	-4.166677
40	1	0	-1.990289	0.714349	-4.570099
41	6	0	-2.866507	-2.783309	-2.764570
42	6	0	-2.431086	-1.554128	-3.280716
43	6	0	-4.157708	-2.863206	-2.220910
44	6	0	-3.242335	-0.410016	-3.245553
45	1	0	-1.439180	-1.487399	-3.722121
46	6	0	-4.984219	-1.738338	-2.194839
47	1	0	-4.515125	-3.810055	-1.822877
48	6	0	-4.529776	-0.517678	-2.698333
49	1	0	-5.981895	-1.811948	-1.772532
50	1	0	-5.176320	0.356245	-2.674099
51	8	0	0.234168	-0.538745	4.422959
52	16	0	-0.345498	-1.059196	3.197023
53	8	0	0.044879	-2.381826	2.737230
54	7	0	-0.275856	0.075188	2.010247
55	6	0	-2.755503	-2.150071	2.969145
56	1	0	-2.147478	-2.758869	2.287520
57	8	0	-2.004041	-1.109489	3.551684
58	1	0	-3.155792	-2.789898	3.766031
59	6	0	-3.938253	-1.587505	2.184924
60	6	0	-0.533862	2.440959	3.083502
61	6	0	-1.085524	3.007541	1.823738
62	1	0	-1.235575	0.349079	1.782204
63	1	0	-2.068348	2.562108	1.597847
64	1	0	-0.424926	2.780312	0.972328
65	6	0	-1.271618	4.543771	1.931330
66	1	0	-0.285370	5.012401	2.061230
67	6	0	0.921952	2.536829	3.332295
68	1	0	1.204655	3.562078	3.635584
69	1	0	1.237526	1.859635	4.133134
70	1	0	1.481580	2.296636	2.418765
71	6	0	-1.459932	2.192333	4.213601
72	1	0	-1.585804	3.107777	4.820420
73	1	0	-2.460400	1.897219	3.871661
74	1	0	-1.074994	1.419974	4.888297
75	1	0	-1.848760	4.766354	2.840569
76	6	0	-1.969362	5.117170	0.733926

77	6	0	-3.366770	5.131517	0.667110
78	6	0	-1.246775	5.598136	-0.361884
79	6	0	-4.023850	5.611475	-0.461182
80	1	0	-3.943284	4.759360	1.515402
81	6	0	-1.900131	6.077778	-1.494099
82	1	0	-0.156891	5.604399	-0.318398
83	6	0	-3.291503	6.083537	-1.548490
84	1	0	-5.112315	5.618303	-0.491761
85	1	0	-1.318961	6.449198	-2.337433
86	1	0	-3.803432	6.459671	-2.432806
87	17	0	-3.370774	-0.661800	0.773453
88	17	0	-4.942532	-0.540759	3.227200
89	17	0	-4.915792	-2.992253	1.639622
90	6	0	-2.966694	2.268600	-1.624417
91	1	0	-2.458228	2.889017	-0.879405
92	1	0	-3.736305	2.882650	-2.105954
93	1	0	-3.456244	1.443584	-1.099224
94	6	0	-1.303463	2.961722	-3.374966
95	1	0	-2.062839	3.574477	-3.873757
96	1	0	-0.794502	3.597095	-2.640119
97	1	0	-0.574064	2.621148	-4.114646
98	6	0	-1.903560	-4.390476	-0.265250
99	1	0	-2.466060	-5.319627	-0.413664
100	1	0	-1.278271	-4.499503	0.626700
101	1	0	-2.615456	-3.579676	-0.082184
102	6	0	-0.032665	-5.240568	-1.726723
103	1	0	0.605233	-5.375986	-0.846379
104	1	0	-0.568188	-6.179285	-1.905074
105	1	0	0.604188	-5.027352	-2.589503
106	6	0	2.299334	4.200027	-0.416563
107	1	0	2.833804	5.147438	-0.285231
108	1	0	1.652442	4.291098	-1.297309
109	1	0	1.667958	4.025631	0.461973
110	6	0	4.186065	3.293732	-1.823161
111	1	0	3.576227	3.388690	-2.725927
112	1	0	4.756727	4.219842	-1.689406
113	1	0	4.884943	2.468720	-1.981662
114	6	0	3.490753	-3.963776	1.463949
115	1	0	2.982276	-4.612230	0.741192
116	1	0	4.244012	-4.563629	1.986372
117	1	0	2.751957	-3.607833	2.187338
118	6	0	5.172867	-3.292838	-0.292660
119	1	0	5.948462	-3.887376	0.203676
120	1	0	4.671676	-3.923382	-1.032377
121	1	0	5.649411	-2.469875	-0.831350

R-^{1}PC$_T$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.617790	-0.591142	-2.117894
2	45	0	0.625605	-0.258716	0.063432
3	8	0	2.999894	-1.850002	-1.237101
4	6	0	2.945368	-2.062188	0.039909
5	8	0	2.078175	-1.511989	0.839173
6	8	0	2.850064	1.026885	-1.762482
7	6	0	2.754868	1.672610	-0.648084
8	8	0	1.905075	1.381231	0.296200
9	8	0	-0.813273	0.943761	-0.827573
10	6	0	-0.738184	1.191028	-2.101025
11	8	0	0.172051	0.701713	-2.885223
12	8	0	0.375970	-2.228609	-2.394375
13	6	0	-0.471855	-2.534839	-1.458901
14	8	0	-0.612888	-1.871169	-0.356202
15	6	0	3.938507	-3.025956	0.670207
16	6	0	4.687167	-2.281894	1.820915
17	1	0	3.949970	-2.046135	2.597047
18	1	0	5.401928	-2.997930	2.246958
19	6	0	5.389734	-1.024054	1.384361
20	6	0	4.695401	0.193677	1.388779
21	6	0	6.718041	-1.036482	0.932418
22	6	0	5.282969	1.379614	0.927585
23	1	0	3.672362	0.215363	1.756904
24	6	0	7.324879	0.140348	0.487826
25	1	0	7.276393	-1.969722	0.937008
26	6	0	6.611168	1.340776	0.477788
27	1	0	8.356503	0.122313	0.149708
28	1	0	7.085792	2.255533	0.129997
29	6	0	3.661590	2.872084	-0.413718
30	6	0	4.473197	2.648133	0.901067
31	1	0	5.123606	3.524780	1.021422
32	1	0	3.762056	2.650528	1.736117
33	6	0	-1.340945	-3.765772	-1.676917
34	6	0	-1.768403	2.130272	-2.712146
35	6	0	-2.169756	-3.560650	-2.983449
36	1	0	-1.464614	-3.538350	-3.822289
37	1	0	-2.799881	-4.451840	-3.103048
38	6	0	-2.513501	1.372042	-3.855244
39	1	0	-3.251231	2.071598	-4.269434
40	1	0	-1.782439	1.155009	-4.642562
41	6	0	-3.009714	-2.311549	-2.988054

42	6	0	-2.456055	-1.105806	-3.441759
43	6	0	-4.330621	-2.308254	-2.515955
44	6	0	-3.179295	0.095249	-3.413047
45	1	0	-1.437652	-1.101817	-3.823869
46	6	0	-5.071746	-1.124456	-2.498236
47	1	0	-4.777429	-3.237070	-2.168026
48	6	0	-4.500114	0.071671	-2.938699
49	1	0	-6.096282	-1.133416	-2.137810
50	1	0	-5.079890	0.991614	-2.922662
51	8	0	0.059881	-1.122697	4.353510
52	16	0	-0.640832	-1.335578	3.110570
53	8	0	-0.399711	-2.491143	2.282277
54	7	0	-0.550863	0.092308	2.171875
55	6	0	-3.142168	-2.211122	2.820124
56	1	0	-2.599448	-2.857846	2.119840
57	8	0	-2.265503	-1.344176	3.518602
58	1	0	-3.659192	-2.825736	3.565383
59	6	0	-4.202084	-1.424321	2.045097
60	6	0	-0.481511	1.439192	2.912928
61	6	0	-0.863499	2.454456	1.822500
62	1	0	-1.413117	0.088455	1.612917
63	1	0	-1.865850	2.198317	1.440647
64	1	0	-0.180012	2.344708	0.972216
65	6	0	-0.872800	3.920088	2.269016
66	1	0	0.156168	4.257205	2.458548
67	6	0	0.944621	1.651856	3.394199
68	1	0	1.024986	2.637313	3.868647
69	1	0	1.237792	0.902523	4.133735
70	1	0	1.637739	1.614854	2.547475
71	6	0	-1.491553	1.507138	4.056849
72	1	0	-1.405817	2.478345	4.555205
73	1	0	-2.520764	1.405872	3.688952
74	1	0	-1.319557	0.743262	4.817798
75	1	0	-1.417621	4.028565	3.216613
76	6	0	-1.520545	4.793183	1.229458
77	6	0	-2.910705	4.949122	1.207960
78	6	0	-0.768559	5.412153	0.228119
79	6	0	-3.531996	5.698069	0.213575
80	1	0	-3.510591	4.467455	1.982304
81	6	0	-1.385718	6.159558	-0.772251
82	1	0	0.316344	5.308548	0.236735
83	6	0	-2.770448	6.302941	-0.784134
84	1	0	-4.615299	5.808635	0.216428
85	1	0	-0.780608	6.632444	-1.544963
86	1	0	-3.254731	6.886713	-1.565111

87	17	0	-3.470328	-0.533206	0.677438
88	17	0	-5.032052	-0.274589	3.126222
89	17	0	-5.371109	-2.619856	1.413777
90	6	0	-2.755120	2.628379	-1.655833
91	1	0	-2.239539	3.189501	-0.870551
92	1	0	-3.484771	3.298232	-2.126182
93	1	0	-3.296867	1.802716	-1.184276
94	6	0	-1.009753	3.324034	-3.322807
95	1	0	-1.722750	4.015789	-3.785819
96	1	0	-0.468218	3.874455	-2.544506
97	1	0	-0.294173	2.986854	-4.077773
98	6	0	-2.259356	-3.997910	-0.475972
99	1	0	-2.867506	-4.894738	-0.643295
100	1	0	-1.668391	-4.137284	0.435229
101	1	0	-2.930178	-3.146920	-0.321488
102	6	0	-0.411139	-4.977062	-1.873293
103	1	0	0.173056	-5.168888	-0.966997
104	1	0	-1.009561	-5.869531	-2.087058
105	1	0	0.279739	-4.805621	-2.703050
106	6	0	2.759412	4.103305	-0.212125
107	1	0	3.375188	4.993136	-0.039973
108	1	0	2.136373	4.283139	-1.096341
109	1	0	2.103514	3.954771	0.652721
110	6	0	4.597468	3.082726	-1.603884
111	1	0	4.029468	3.241930	-2.524348
112	1	0	5.227232	3.961357	-1.422937
113	1	0	5.242039	2.214091	-1.760858
114	6	0	3.136338	-4.187291	1.288786
115	1	0	2.628376	-4.765301	0.509334
116	1	0	3.816715	-4.861663	1.820772
117	1	0	2.384417	-3.811617	1.989069
118	6	0	4.924087	-3.552358	-0.372892
119	1	0	5.632084	-4.237783	0.107533
120	1	0	4.401576	-4.092557	-1.166850
121	1	0	5.484505	-2.738304	-0.839787