Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Remote N-H Activation of Indole Aldehyde: An Investigation on Mechanism, Origin of Selectivities, and Role of the Catalyst

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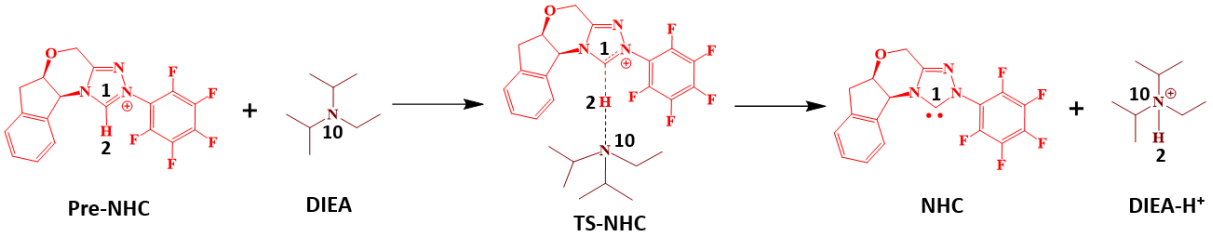
Content

SI 1. Generation of Active Catalyst NHC



Scheme S1. Schematic representation for the generation of **NHC** in presence of **DIEA**.

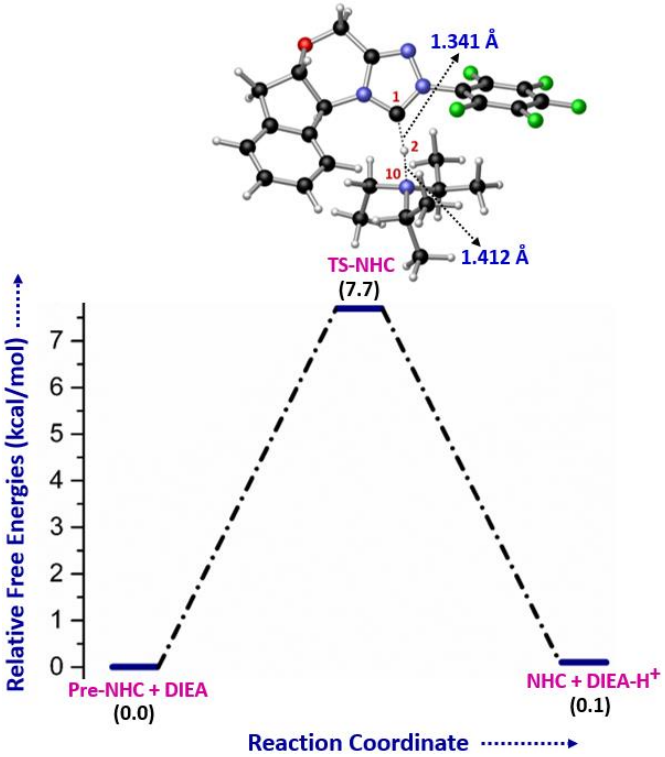


Figure S1. The relative free energy plot for the generation of active catalyst **NHC**.

SI 2. Computational Equation for the Calculation of Enantiomeric Excess (ee)

The reported enantiomeric excess (ee) value has been calculated by adopting the following mentioned Boltzmann distribution equation:

$$\frac{[\boldsymbol{Si}\text{-TS7}]}{[\boldsymbol{Re}\text{-TS7}]} = \frac{e^{-G^{\neq}_{[\boldsymbol{Re}\text{-TS7}]}/\mathrm{RT}}}{e^{-G^{\neq}_{[\boldsymbol{Si}\text{-TS7}]}/\mathrm{RT}}} = e^{\Delta G^{\neq}/\mathrm{RT}} \qquad [1]$$

$$\text{ee}\% = \frac{[\boldsymbol{Si}\text{-TS7}]-[\boldsymbol{Re}\text{-TS7}]}{[\boldsymbol{Si}\text{-TS7}]+[\boldsymbol{Re}\text{-TS7}]} \times 100\% = \frac{\frac{[\boldsymbol{Si}\text{-TS7}]}{[\boldsymbol{Re}\text{-TS7}]}-1}{\frac{[\boldsymbol{Si}\text{-TS7}]}{[\boldsymbol{Re}\text{-TS7}]}+1} \times 100\% \qquad [2]$$

The $\Delta G^{\neq}$ used in the above equation is the relative Gibb's free energy difference between the two stereo-selective transition states, ***Si*-TS7** and ***Re*-TS7**.

The **Figure 6** in the main text reflects that the relative Gibbs free energy barriers for the two competing stereo-selective transition states, ***Si*-TS7** and ***Re*-TS7** are 21.5 and 26.8 kcal/mol, respectively. Thus, the value of $\Delta G^{\neq}$ is evaluated to be 5.3 kcal/mol (22175.2 J/mol). Knowing

the value of $\Delta G^{\neq}$ and using the **Eq-1**, the energy ratio $\frac{[Si-\mathbf{TS7}]}{[Re-\mathbf{TS7}]}$ of the two competing stereo-selective transition states has been evaluated to be 7676.14. This in turn gives an enantiomeric excess (ee %) value of 99.9%, which is in close proximity to the experimentally determined value.

SI 3. Lowest Energy Geometries of Some Stationery Points Optimised at M06-2X/6-31G(d,p)//IEF-PCM$_{DCM}$ Level of Theory

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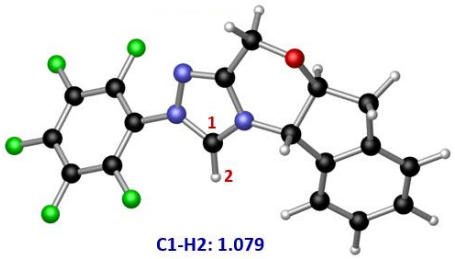
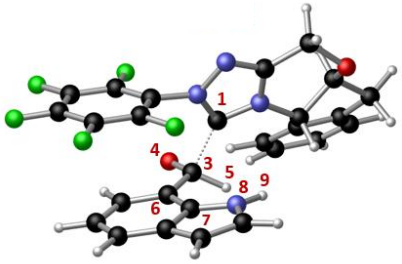
<tr><td> 
</td><td> 
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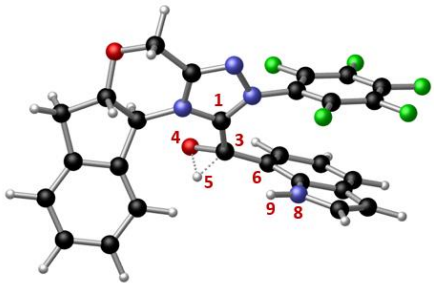
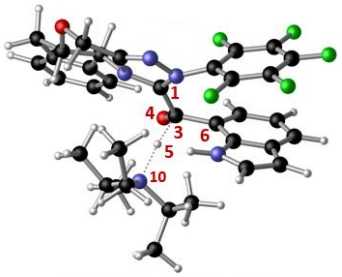
<tr><td>Pre-NHC</td><td>Si-TS1</td></tr>
<tr><td> 
</td><td> 
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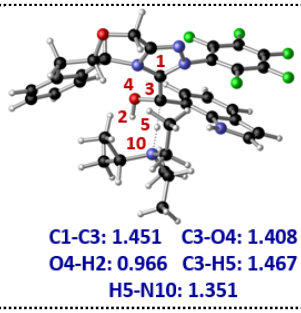
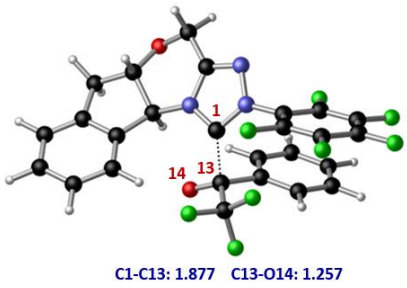
<tr><td>TS2</td><td>TS3</td></tr>
<tr><td> 
</td><td> 
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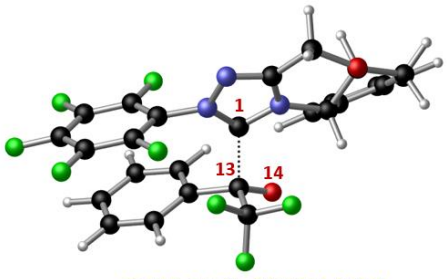
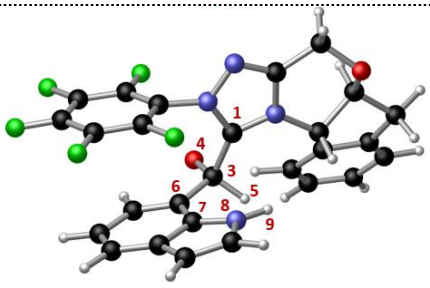
<tr><td>TS4</td><td>Si-TS1′</td></tr>
<tr><td> 
</td><td> 
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<tr><td>Re-TS1′</td><td>Si-INT1</td></tr>
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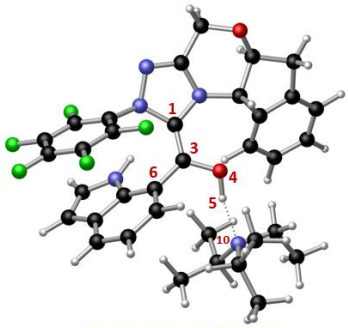
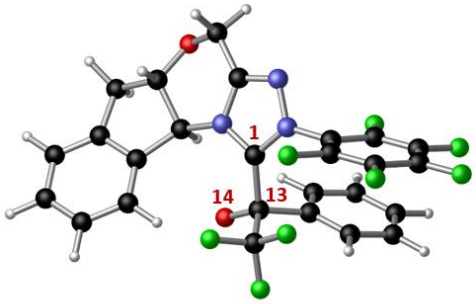
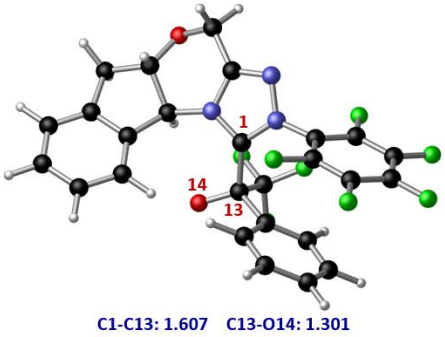


INT4



Si-INT1′



Re-INT1′

Figure S2. DFT optimized geometries of some stationary points along with their bond distances (unit: Å).

SI 4. Absolute Energies of All the DFT Optimized Stationary Points Involved in this Mechanistic Investigation

Table S1. DFT derived energies $\mathbf{E_1}$ and $\mathbf{E_2}$ of all the optimised stationary points involved in this work, obtained at M06-2X/6-31G(d,p)//IEF-PCM$_{(DCM)}$ (L_1) and M06-2X/6-311++G(2df,2pd)//IEF-PCM$_{(DCM)}$ (L_2) levels, respectively at 298.15 K temperature

Stationary Point	E_1	E_2
Pre-NHC	-1430.44998318	-1430.93793924
TS-NHC	-1801.32467079	-1801.91820155
NHC	-1429.98908408	-1430.48459587
R1	-476.962674250	-477.114914724
R2	-682.364253323	-682.606994919
DIEA	-370.859431171	-370.970195353
DIEA-H$^+$	-371.318012517	-371.424441435
DQ	-1240.99733330	-1241.36431308
DQ-H$^-$	-1241.74658753	-1242.12421132
***Si*-TS1**	-1906.95311604	-1907.59811203
***Re*-TS1**	-1906.95802416	-1907.60347936

TS2	-1906.88685893	-1907.53574395
TS3	-2277.79049749	-2278.53786126
TS4	-2278.27417074	-2279.01407946
TS5	-2,649.16550214	-2650.00967589
TS6	-3147.96660380	-3148.97147047
TS7	-2277.10177886	-2277.83963596
***Re*-TS8**	-2588.13203096	-2589.00908927
***Si*-TS8**	-2588.13887503	-2589.01731060
***Re*-TS9**	-2588.17043383	-2589.04367256
***Si*-TS9**	-2588.17000558	-2589.04347604
***Si*-INT1**	-1906.96023891	-1907.60739512
***Re*-INT1**	-1906.96134041	-1907.60813042
INT2	-1906.97792255	-1907.62245671
INT3	-2278.32746150	-2279.06948126
INT4	-2277.87440761	-2278.62600844
INT5	-1906.22521313	-1906.85869536
INT6	-1905.75726876	-1906.39965017
***Re*-INT7**	-2588.17970127	-2589.05324527
***Si*-INT7**	-2588.17931240	-2589.05210428
***R*-P**	-1158.16615557	-1158.55142893
***S*-P**	-1158.16521162	-1158.55135873
***Si*-TS1′**	-2112.36201697	-2113.09485783
***Re*-TS1′**	-2112.36054637	-2113.09435946
***Si*-INT1′**	-2112.36426747	-2113.09806106
***Re*-INT1′**	-2112.36332095	-2113.09831897

SI 5. Cartesian Co-ordinates of All the Optimized Stationary Points Involved in the NHC catalysed N-H activation of indole aldehyde, Evaluated at M06-2X/6-31G(d,p)//IEF-PCM$_{(DCM)}$ Level of Theory

Pre-NHC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.542715	-0.405649	-1.801447
2	6	0	-0.471064	1.737287	-2.176126

3	7	0	-0.498890	1.188374	-3.356147
4	7	0	-0.492645	0.773749	-1.189337
5	7	0	-0.537739	-0.147560	-3.105022
6	6	0	-0.361414	3.214546	-1.869926
7	1	0	-1.131205	3.754164	-2.422890
8	1	0	0.625764	3.552508	-2.211932
9	8	0	-0.538730	3.483919	-0.492879
10	6	0	0.163958	2.541662	0.280188
11	1	0	1.179142	2.404264	-0.126135
12	6	0	-0.545561	1.183915	0.223592
13	1	0	-1.608066	1.321922	0.458340
14	6	0	0.278468	2.796475	1.777644
15	1	0	1.053263	3.521422	2.029832
16	1	0	-0.679476	3.152669	2.174788
17	6	0	0.584360	1.386294	2.252265
18	6	0	0.153232	0.425759	1.321060
19	6	0	1.205351	0.983836	3.425805
20	1	0	1.549342	1.718319	4.147134
21	6	0	0.322240	-0.931159	1.554591
22	1	0	-0.027977	-1.683522	0.855816
23	6	0	1.392238	-0.379775	3.657544
24	1	0	1.883075	-0.706628	4.568206
25	6	0	0.958081	-1.327193	2.732193
26	1	0	1.110404	-2.382881	2.928399
27	6	0	-0.595234	-1.078954	-4.171615
28	6	0	-1.534219	-2.105870	-4.149137
29	6	0	0.271727	-0.954654	-5.254388
30	6	0	-1.608458	-3.010129	-5.196726
31	6	0	0.189266	-1.848651	-6.311525
32	6	0	-0.747432	-2.875032	-6.279290
33	9	0	1.180274	0.005835	-5.280388
34	9	0	1.012688	-1.735457	-7.342792
35	9	0	-0.816041	-3.732191	-7.282411
36	9	0	-2.499619	-3.989457	-5.171956
37	9	0	-2.355522	-2.225052	-3.112343
38	1	0	-0.582907	-1.384864	-1.349134

TS-NHC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.391591	-3.002401	-2.148227
2	6	0	-1.096856	-0.909220	-2.387314
3	7	0	-1.048020	-1.374943	-3.598230
4	7	0	-0.669826	-1.862700	-1.484488
5	7	0	-0.605360	-2.657062	-3.426272
6	6	0	-1.551595	0.471213	-1.967857
7	1	0	-2.504045	0.693113	-2.450560
8	1	0	-0.803965	1.202395	-2.301951
9	8	0	-1.740065	0.552240	-0.565864
10	6	0	-0.627850	-0.019992	0.074240
11	1	0	0.296942	0.336018	-0.408489
12	6	0	-0.656203	-1.546827	-0.057838
13	1	0	-1.597211	-1.918548	0.368766
14	6	0	-0.468047	0.162495	1.582779
15	1	0	-0.116916	1.156074	1.863543
16	1	0	-1.420010	-0.033202	2.090824
17	6	0	0.553148	-0.935514	1.842368
18	6	0	0.506952	-1.906658	0.827902
19	6	0	1.505767	-1.036136	2.846178

20	1	0	1.561486	-0.289760	3.632454
21	6	0	1.426483	-2.939317	0.771008
22	1	0	1.423146	-3.645876	-0.051874
23	6	0	2.414017	-2.098375	2.813878
24	1	0	3.166051	-2.182935	3.591236
25	6	0	2.387169	-3.031934	1.780109
26	1	0	3.120501	-3.831069	1.750517
27	6	0	-0.345138	-3.466463	-4.555971
28	6	0	-1.382088	-3.861360	-5.395166
29	6	0	0.958179	-3.870642	-4.829731
30	6	0	-1.125250	-4.683406	-6.482275
31	6	0	1.222394	-4.697818	-5.911390
32	6	0	0.177717	-5.097503	-6.737189
33	9	0	1.950166	-3.491951	-4.033725
34	9	0	2.460298	-5.094936	-6.166510
35	9	0	0.424746	-5.883276	-7.771084
36	9	0	-2.111727	-5.076880	-7.274482
37	9	0	-2.624056	-3.479578	-5.135215
38	1	0	-0.343415	-4.270046	-1.712452
39	6	0	-1.464928	-4.969911	-0.004691
40	1	0	-2.214388	-4.307868	-0.449008
41	6	0	0.609764	-6.172582	-0.606630
42	1	0	0.786037	-5.683834	0.357764
43	6	0	1.820797	-5.867820	-1.493984
44	1	0	1.868494	-4.814563	-1.786238
45	1	0	2.733130	-6.101061	-0.938255
46	1	0	1.829611	-6.465930	-2.407071
47	6	0	0.502377	-7.672957	-0.322483
48	1	0	1.398533	-7.977744	0.223803
49	1	0	-0.363869	-7.923959	0.290872
50	1	0	0.459588	-8.269174	-1.235840
51	6	0	-1.465014	-6.362930	-2.058016
52	1	0	-1.763608	-7.269406	-1.517444
53	6	0	-2.734890	-5.626519	-2.491647
54	1	0	-3.229326	-6.206239	-3.273861
55	1	0	-3.452214	-5.498685	-1.679041
56	1	0	-2.508622	-4.639264	-2.908516
57	6	0	-0.672931	-6.787164	-3.294036
58	1	0	-0.237253	-5.922765	-3.799470
59	1	0	0.129853	-7.487986	-3.071413
60	1	0	-1.350652	-7.280962	-3.994328
61	7	0	-0.647233	-5.517731	-1.125123
62	6	0	-2.142960	-5.971836	0.921312
63	1	0	-2.768067	-6.683827	0.375724
64	1	0	-1.416524	-6.527400	1.517319
65	1	0	-2.787985	-5.424851	1.612701
66	1	0	-0.795083	-4.333228	0.582315

NHC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.580398	-0.469657	-1.728985
2	6	0	-0.505558	1.754360	-2.176825
3	7	0	-0.544878	1.208565	-3.350138
4	7	0	-0.513493	0.782690	-1.195219
5	7	0	-0.585046	-0.141267	-3.046856
6	6	0	-0.389288	3.231157	-1.872832
7	1	0	-1.157924	3.782890	-2.415973
8	1	0	0.596476	3.575037	-2.215036

9	8	0	-0.553740	3.513658	-0.490430
10	6	0	0.144597	2.559821	0.276321
11	1	0	1.163219	2.433414	-0.127399
12	6	0	-0.553321	1.201717	0.194144
13	1	0	-1.607021	1.343066	0.473745
14	6	0	0.251340	2.797296	1.780089
15	1	0	1.012608	3.530128	2.052902
16	1	0	-0.715309	3.133605	2.175484
17	6	0	0.575455	1.382223	2.234239
18	6	0	0.157382	0.440338	1.278921
19	6	0	1.215142	0.957898	3.390153
20	1	0	1.553147	1.675466	4.131889
21	6	0	0.371957	-0.917948	1.455140
22	1	0	0.049108	-1.623014	0.696545
23	6	0	1.434480	-0.409502	3.575469
24	1	0	1.940026	-0.753516	4.472238
25	6	0	1.022874	-1.335959	2.618296
26	1	0	1.211364	-2.392649	2.777882
27	6	0	-0.629075	-1.064680	-4.109925
28	6	0	-1.615800	-2.045935	-4.164409
29	6	0	0.316023	-1.011099	-5.131781
30	6	0	-1.650790	-2.960085	-5.208288
31	6	0	0.275663	-1.909065	-6.188169
32	6	0	-0.707218	-2.888244	-6.223307
33	9	0	1.283377	-0.101844	-5.102514
34	9	0	1.186462	-1.846600	-7.154954
35	9	0	-0.744424	-3.756515	-7.226831
36	9	0	-2.598405	-3.892097	-5.248532
37	9	0	-2.549616	-2.117744	-3.223943

R1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.909814	0.681585	-0.710207
2	6	0	-4.130308	1.870479	0.035243
3	6	0	-5.432556	2.187151	0.442479
4	6	0	-6.480371	1.336497	0.111223
5	6	0	-6.248154	0.168341	-0.623098
6	6	0	-4.968215	-0.183757	-1.047313
7	1	0	-5.619413	3.092679	1.012034
8	1	0	-7.490129	1.579000	0.424028
9	1	0	-7.067061	-0.495402	-0.881356
10	6	0	-2.852255	2.505513	0.197873
11	1	0	-2.647668	3.431030	0.714256
12	6	0	-1.937356	1.712255	-0.429805
13	1	0	-0.869690	1.831742	-0.539787
14	7	0	-2.568101	0.614152	-0.977757
15	1	0	-2.096828	-0.113945	-1.490430
16	6	0	-4.755736	-1.419998	-1.816767
17	1	0	-3.710280	-1.631665	-2.117120
18	8	0	-5.641259	-2.191667	-2.126316

R2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.672062	-2.285930	-0.010843
2	6	0	-1.272148	-2.293651	0.005947

3	6	0	-0.563512	-1.086093	0.011390
4	6	0	-1.247640	0.120647	0.000283
5	6	0	-2.643084	0.126465	-0.016504
6	6	0	-3.351766	-1.072968	-0.022064
7	1	0	-3.233118	-3.212886	-0.015249
8	1	0	0.520741	-1.116913	0.024614
9	1	0	-0.698543	1.055895	0.004688
10	1	0	-3.179626	1.069716	-0.025384
11	1	0	-4.436057	-1.064302	-0.035272
12	6	0	-0.478652	-3.544224	0.018779
13	8	0	0.729067	-3.586199	0.032096
14	6	0	-1.244011	-4.888162	0.015861
15	9	0	-0.403152	-5.914098	0.028918
16	9	0	-2.039984	-4.982132	1.089921
17	9	0	-2.017094	-4.990678	-1.073995

DIEA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.357194	1.636393	-0.851499
2	1	0	-0.249669	2.557219	-0.260085
3	1	0	-1.247586	1.793949	-1.466548
4	6	0	0.862230	1.458703	-1.747567
5	1	0	0.730992	0.585682	-2.393214
6	1	0	1.028945	2.339465	-2.375112
7	1	0	1.759849	1.294642	-1.142747
8	6	0	0.001791	0.774652	1.368856
9	1	0	0.882364	1.392415	1.150894
10	6	0	0.557669	-0.446813	2.108300
11	1	0	1.106076	-1.085341	1.410869
12	1	0	1.249071	-0.111376	2.887640
13	1	0	-0.213291	-1.046866	2.593724
14	6	0	-0.918640	1.617636	2.261148
15	1	0	-0.386329	1.932637	3.163544
16	1	0	-1.258404	2.517388	1.738783
17	1	0	-1.803663	1.058197	2.576397
18	6	0	-1.909881	-0.076919	-0.070101
19	1	0	-2.664274	0.713661	0.108309
20	6	0	-2.118462	-0.637969	-1.481978
21	1	0	-3.136940	-1.022006	-1.588527
22	1	0	-1.959461	0.102812	-2.268187
23	1	0	-1.416012	-1.461300	-1.647096
24	6	0	-2.183500	-1.216400	0.910898
25	1	0	-1.426995	-1.999729	0.800872
26	1	0	-2.204224	-0.895192	1.952415
27	1	0	-3.160242	-1.652251	0.682907
28	7	0	-0.547762	0.473034	0.031524

DIEA-H$^+$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.337726	1.640421	-0.897772
2	1	0	-0.297315	2.519898	-0.255687
3	1	0	-1.218447	1.735820	-1.528183
4	6	0	0.925026	1.492581	-1.725031
5	1	0	0.852981	0.639880	-2.405926
6	1	0	1.066845	2.393337	-2.324172

7	1	0	1.809110	1.367497	-1.093180
8	6	0	0.042669	0.779384	1.399087
9	1	0	0.903953	1.405214	1.147569
10	6	0	0.584729	-0.440801	2.133455
11	1	0	1.200396	-1.063550	1.478189
12	1	0	1.230010	-0.076320	2.935932
13	1	0	-0.190508	-1.057318	2.585171
14	6	0	-0.938428	1.608144	2.213851
15	1	0	-0.415698	1.963012	3.104225
16	1	0	-1.296633	2.484766	1.668976
17	1	0	-1.799894	1.026373	2.544899
18	6	0	-1.950209	-0.113777	-0.063791
19	1	0	-2.595848	0.740774	0.159274
20	6	0	-2.201916	-0.629223	-1.479811
21	1	0	-3.239848	-0.960380	-1.541087
22	1	0	-2.051219	0.115011	-2.261551
23	1	0	-1.564512	-1.493978	-1.691523
24	6	0	-2.194261	-1.245195	0.926650
25	1	0	-1.465492	-2.050348	0.792255
26	1	0	-2.188120	-0.924116	1.966263
27	1	0	-3.183593	-1.657317	0.718014
28	7	0	-0.527595	0.437660	0.014345
29	1	0	0.075012	-0.307418	-0.354335

DQ

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.428851	2.142552	-0.095275
2	6	0	-3.310686	0.797297	-0.118656
3	6	0	-2.038731	0.098506	-0.044701
4	6	0	-0.846697	0.925759	0.037533
5	6	0	-0.873024	2.275293	0.086506
6	6	0	-2.193480	2.970128	0.039708
7	1	0	-4.207506	0.206575	-0.232623
8	1	0	0.110280	0.429674	0.102088
9	6	0	-1.966490	-1.287057	-0.044001
10	6	0	-0.694528	-1.985940	-0.117043
11	6	0	-3.158551	-2.114212	0.038859
12	6	0	-0.576385	-3.331169	-0.092232
13	1	0	0.202318	-1.395352	-0.231505
14	6	0	-3.132248	-3.463692	0.089237
15	1	0	-4.115533	-1.618038	0.102700
16	6	0	-1.811792	-4.158589	0.043370
17	6	0	-4.779033	2.851135	-0.200949
18	6	0	-4.786088	3.788452	-1.424262
19	1	0	-5.770065	4.260445	-1.513017
20	1	0	-4.031792	4.569521	-1.331098
21	1	0	-4.598558	3.222230	-2.342438
22	6	0	-5.928467	1.850914	-0.370754
23	1	0	-6.006821	1.170590	0.483699
24	1	0	-6.870358	2.401692	-0.443600
25	1	0	-5.818876	1.255698	-1.283285
26	6	0	-5.045865	3.660198	1.083087
27	1	0	-4.290226	4.430953	1.231427
28	1	0	-6.027132	4.140776	1.010191
29	1	0	-5.055494	3.000474	1.956658
30	6	0	0.396901	3.118306	0.200979
31	6	0	0.506153	4.064693	-1.010106
32	1	0	0.528863	3.492143	-1.942999

33	1	0	-0.329312	4.763458	-1.044965
34	1	0	1.437941	4.635556	-0.940601
35	6	0	1.654658	2.241202	0.224028
36	1	0	2.535203	2.885513	0.297219
37	1	0	1.664529	1.565649	1.085673
38	1	0	1.752571	1.645264	-0.689489
39	6	0	0.369853	3.935595	1.506952
40	1	0	0.303672	3.270289	2.373910
41	1	0	1.297328	4.511509	1.592425
42	1	0	-0.472883	4.626179	1.526431
43	6	0	-4.402198	-4.306579	0.204343
44	6	0	-5.659949	-3.429436	0.226235
45	1	0	-6.540516	-4.073667	0.299879
46	1	0	-5.670004	-2.753026	1.087205
47	1	0	-5.757653	-2.834411	-0.687897
48	6	0	-4.375416	-5.122498	1.511175
49	1	0	-5.302967	-5.698218	1.597126
50	1	0	-3.532760	-5.813157	1.531502
51	1	0	-4.309281	-4.456292	2.377446
52	6	0	-4.511247	-5.254228	-1.005774
53	1	0	-4.533730	-4.682652	-1.939271
54	1	0	-3.675817	-5.953076	-1.039723
55	1	0	-5.443086	-5.824959	-0.935867
56	6	0	0.773802	-4.039877	-0.196983
57	6	0	1.923279	-3.039833	-0.367506
58	1	0	2.001482	-2.358694	0.486313
59	1	0	2.865176	-3.590694	-0.439651
60	1	0	1.813868	-2.445488	-1.280623
61	6	0	0.781062	-4.978311	-1.419437
62	1	0	0.026717	-5.759262	-1.325704
63	1	0	0.593740	-4.412931	-2.338172
64	1	0	1.765036	-5.450431	-1.507565
65	6	0	1.040388	-4.847779	1.087835
66	1	0	1.049869	-4.187267	1.960812
67	1	0	0.284711	-5.618392	1.236724
68	1	0	2.021664	-5.328435	1.015551
69	8	0	-2.261908	4.193979	0.109954
70	8	0	-1.743396	-5.382373	0.114840

DQ-H$^-$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.364930	2.203478	-0.358883
2	6	0	-3.246290	0.814105	-0.361263
3	6	0	-2.059685	0.147096	-0.033208
4	6	0	-0.954578	0.939306	0.292658
5	6	0	-0.992591	2.335371	0.293464
6	6	0	-2.217687	2.953566	-0.028677
7	1	0	-4.100005	0.211491	-0.646388
8	1	0	-0.039774	0.434125	0.576673
9	6	0	-1.978666	-1.329230	-0.027269
10	6	0	-0.787942	-1.999464	-0.341849
11	6	0	-3.086600	-2.124235	0.300650
12	6	0	-0.669396	-3.382261	-0.336679
13	1	0	0.068971	-1.396103	-0.628751
14	6	0	-3.046287	-3.511399	0.324259
15	1	0	-4.006762	-1.616036	0.575812
16	6	0	-1.813935	-4.209035	0.002156
17	6	0	-4.695265	2.887770	-0.714393

18	6	0	-4.528092	3.781621	-1.956820
19	1	0	-5.489312	4.242576	-2.211202
20	1	0	-3.798037	4.573133	-1.789716
21	1	0	-4.203593	3.182522	-2.814003
22	6	0	-5.790104	1.862562	-1.040746
23	1	0	-5.993134	1.198728	-0.194337
24	1	0	-6.716039	2.395394	-1.278082
25	1	0	-5.526735	1.247572	-1.906818
26	6	0	-5.198603	3.724717	0.476401
27	1	0	-4.492501	4.510861	0.743901
28	1	0	-6.157881	4.189233	0.221478
29	1	0	-5.355364	3.083647	1.350258
30	6	0	0.260462	3.155612	0.654679
31	6	0	0.686977	4.050667	-0.530095
32	1	0	0.961532	3.422533	-1.382541
33	1	0	-0.082933	4.740391	-0.885662
34	1	0	1.560822	4.647440	-0.249650
35	6	0	1.467201	2.253482	0.953793
36	1	0	2.332792	2.881737	1.184553
37	1	0	1.284445	1.605266	1.815445
38	1	0	1.725095	1.626671	0.095311
39	6	0	0.022759	3.983227	1.936578
40	1	0	-0.182652	3.309688	2.773663
41	1	0	0.918759	4.564623	2.176216
42	1	0	-0.816981	4.681736	1.884598
43	6	0	-4.287652	-4.332678	0.695985
44	6	0	-5.502780	-3.455144	1.020470
45	1	0	-6.356296	-4.095807	1.268190
46	1	0	-5.315836	-2.801045	1.879064
47	1	0	-5.790679	-2.828039	0.169641
48	6	0	-3.994504	-5.196947	1.935225
49	1	0	-4.868718	-5.809061	2.190411
50	1	0	-3.141004	-5.845056	1.736006
51	1	0	-3.764680	-4.559163	2.796394
52	6	0	-4.676305	-5.243722	-0.482278
53	1	0	-4.962698	-4.638585	-1.350015
54	1	0	-3.829605	-5.874796	-0.752745
55	1	0	-5.532076	-5.875179	-0.211852
56	6	0	0.657498	-4.063238	-0.694158
57	6	0	1.766199	-3.057138	-1.026176
58	1	0	1.975961	-2.388718	-0.183799
59	1	0	2.688873	-3.599064	-1.261321
60	1	0	1.509719	-2.441026	-1.894740
61	6	0	0.470987	-4.967127	-1.925618
62	1	0	-0.313663	-5.698650	-1.733304
63	1	0	0.190364	-4.365628	-2.797705
64	1	0	1.406657	-5.489728	-2.161608
65	6	0	1.142836	-4.911018	0.495579
66	1	0	1.351795	-4.268087	1.358378
67	1	0	0.373866	-5.633642	0.769374
68	1	0	2.068132	-5.440790	0.235950
69	8	0	-2.357920	4.322508	-0.038355
70	8	0	-1.739291	-5.486379	0.016018
71	1	0	-1.529670	4.735828	0.217978

***Si*-TS1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.619951	0.562512	-1.146932

2	6	0	-3.189478	1.674000	-0.380053
3	6	0	-4.065455	2.226865	0.569569
4	6	0	-5.319406	1.660225	0.732315
5	6	0	-5.726865	0.561688	-0.048532
6	6	0	-4.897696	-0.001994	-1.004348
7	1	0	-3.762508	3.085402	1.161337
8	1	0	-6.007550	2.075496	1.462531
9	1	0	-6.715836	0.129069	0.065448
10	6	0	-1.860183	1.994863	-0.820470
11	1	0	-1.229534	2.791987	-0.456108
12	6	0	-1.540235	1.101507	-1.801344
13	1	0	-0.633914	0.998148	-2.379719
14	7	0	-2.599802	0.245182	-2.015083
15	1	0	-2.558682	-0.570941	-2.604234
16	6	0	-5.402084	-1.166347	-1.840615
17	1	0	-4.577268	-1.899240	-2.026358
18	8	0	-6.569441	-1.596000	-1.647655
19	6	0	-5.202707	-0.409861	-3.584990
20	7	0	-4.659488	-0.927740	-4.706100
21	7	0	-5.460747	0.852906	-3.943781
22	6	0	-4.547476	0.073009	-5.656129
23	6	0	-4.071313	-2.242210	-4.964287
24	7	0	-5.051262	1.182393	-5.212378
25	6	0	-6.067197	1.828107	-3.119354
26	6	0	-3.907827	-0.150075	-7.005733
27	6	0	-3.929512	-2.385857	-6.483913
28	1	0	-3.061465	-2.236178	-4.529650
29	6	0	-4.756196	-3.548630	-4.630713
30	6	0	-5.311098	2.888924	-2.634300
31	6	0	-7.392633	1.685826	-2.729121
32	1	0	-3.236797	0.680451	-7.227246
33	1	0	-4.694401	-0.185892	-7.771419
34	8	0	-3.148070	-1.346415	-7.019143
35	1	0	-4.943198	-2.342641	-6.915433
36	6	0	-3.414105	-3.813350	-6.622723
37	6	0	-4.283837	-4.482596	-5.572192
38	6	0	-5.645143	-3.915239	-3.629865
39	6	0	-5.873958	3.805546	-1.761303
40	9	0	-4.037867	3.008714	-2.984188
41	6	0	-7.962791	2.603234	-1.858243
42	9	0	-8.117176	0.673681	-3.181636
43	1	0	-3.545210	-4.227455	-7.623448
44	1	0	-2.349406	-3.854958	-6.360977
45	6	0	-4.673534	-5.810824	-5.492613
46	1	0	-6.062109	-3.194321	-2.926936
47	6	0	-6.036965	-5.256555	-3.567574
48	6	0	-7.199804	3.656950	-1.374382
49	9	0	-5.142838	4.796509	-1.264262
50	9	0	-9.230283	2.472569	-1.480524
51	1	0	-4.317514	-6.534480	-6.219655
52	6	0	-5.549756	-6.194493	-4.475243
53	1	0	-6.736552	-5.568363	-2.798657
54	9	0	-7.738136	4.522927	-0.525978
55	1	0	-5.868747	-7.229386	-4.403185

***Re*-TS1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.303988	-2.682286	-2.188871

2	6	0	-3.126253	-3.945298	-1.567554
3	6	0	-4.256207	-4.653328	-1.124160
4	6	0	-5.510147	-4.088894	-1.294117
5	6	0	-5.660257	-2.828688	-1.902375
6	6	0	-4.572687	-2.109710	-2.371704
7	1	0	-4.143434	-5.628615	-0.659892
8	1	0	-6.391952	-4.624208	-0.956834
9	1	0	-6.644455	-2.384916	-2.022466
10	6	0	-1.715777	-4.218043	-1.569285
11	1	0	-1.222977	-5.095067	-1.176518
12	6	0	-1.106999	-3.151833	-2.169582
13	1	0	-0.061580	-2.969768	-2.370463
14	7	0	-2.054398	-2.229050	-2.552109
15	1	0	-1.850031	-1.350392	-3.001282
16	6	0	-4.781435	-0.760165	-3.041218
17	1	0	-3.799349	-0.293390	-3.279608
18	8	0	-5.740355	-0.031106	-2.657594
19	6	0	-5.260746	-1.310792	-4.757278
20	7	0	-6.281392	-0.682094	-5.379574
21	7	0	-5.299524	-2.538108	-5.301367
22	6	0	-6.917501	-1.580491	-6.214575
23	6	0	-6.874093	0.641797	-5.167243
24	7	0	-6.321569	-2.732170	-6.197797
25	6	0	-4.411190	-3.599036	-5.023175
26	6	0	-8.149150	-1.233820	-7.016626
27	6	0	-7.746891	0.933821	-6.393791
28	1	0	-7.490273	0.563667	-4.264504
29	6	0	-6.062505	1.912728	-5.108957
30	6	0	-4.894622	-4.813232	-4.546481
31	6	0	-3.040716	-3.425465	-5.181498
32	1	0	-8.876054	-2.041225	-6.920394
33	1	0	-7.867758	-1.133886	-8.073985
34	8	0	-8.750225	-0.040697	-6.549600
35	1	0	-7.089148	0.921078	-7.279291
36	6	0	-8.182422	2.374214	-6.158556
37	6	0	-6.870796	2.934138	-5.636686
38	6	0	-4.797947	2.189473	-4.614272
39	6	0	-4.018896	-5.842105	-4.236756
40	9	0	-6.195837	-4.985479	-4.358954
41	6	0	-2.159902	-4.447554	-4.868532
42	9	0	-2.559162	-2.253030	-5.586607
43	1	0	-8.543752	2.871249	-7.060158
44	1	0	-8.969673	2.410258	-5.395443
45	6	0	-6.415516	4.245024	-5.663878
46	1	0	-4.174544	1.403576	-4.207767
47	6	0	-4.338636	3.507106	-4.658088
48	6	0	-2.652016	-5.654982	-4.393308
49	9	0	-4.478880	-6.987225	-3.743330
50	9	0	-0.849254	-4.261829	-4.989017
51	1	0	-7.035408	5.035534	-6.076188
52	6	0	-5.140935	4.525820	-5.169501
53	1	0	-3.346637	3.739868	-4.284734
54	9	0	-1.810334	-6.621846	-4.053431
55	1	0	-4.767849	5.544695	-5.191675

TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.173192	-2.281627	-2.738352

2	6	0	-2.340198	-3.377200	-2.413694
3	6	0	-2.895909	-4.468542	-1.719505
4	6	0	-4.237239	-4.424097	-1.376345
5	6	0	-5.054258	-3.335632	-1.742429
6	6	0	-4.551557	-2.261620	-2.463697
7	1	0	-2.281819	-5.324207	-1.455766
8	1	0	-4.678973	-5.252706	-0.831545
9	1	0	-6.110672	-3.322794	-1.495689
10	6	0	-1.034805	-3.070126	-2.932320
11	1	0	-0.149117	-3.685449	-2.873320
12	6	0	-1.119514	-1.840348	-3.525088
13	1	0	-0.361016	-1.254215	-4.022695
14	7	0	-2.406722	-1.362740	-3.417297
15	1	0	-2.713055	-0.447152	-3.708929
16	6	0	-5.431003	-1.165140	-2.937800
17	1	0	-5.569183	-0.223080	-2.270202
18	8	0	-6.693672	-0.956331	-2.235597
19	6	0	-5.526220	-0.899071	-4.342765
20	7	0	-6.257525	0.107122	-4.905349
21	7	0	-5.023504	-1.566432	-5.417426
22	6	0	-6.249588	-0.080958	-6.271519
23	6	0	-7.124214	1.111850	-4.289743
24	7	0	-5.489877	-1.068286	-6.616899
25	6	0	-4.389887	-2.828644	-5.409300
26	6	0	-7.123739	0.729148	-7.199952
27	6	0	-7.613324	2.044622	-5.406180
28	1	0	-7.965792	0.570146	-3.846607
29	6	0	-6.652393	2.163657	-3.303627
30	6	0	-5.051698	-3.929430	-4.875438
31	6	0	-3.082950	-2.966216	-5.861926
32	1	0	-7.555732	0.059153	-7.943645
33	1	0	-6.521122	1.491443	-7.711320
34	8	0	-8.181061	1.332613	-6.475946
35	1	0	-6.737480	2.602647	-5.776437
36	6	0	-8.480467	3.025182	-4.624251
37	6	0	-7.544610	3.244487	-3.447265
38	6	0	-5.602439	2.236463	-2.399416
39	6	0	-4.396044	-5.141517	-4.733567
40	9	0	-6.302678	-3.801139	-4.449361
41	6	0	-2.425277	-4.179929	-5.741138
42	9	0	-2.437146	-1.916378	-6.356102
43	1	0	-8.706693	3.941747	-5.170871
44	1	0	-9.420719	2.545972	-4.325648
45	6	0	-7.428853	4.365128	-2.639523
46	1	0	-4.854348	1.453457	-2.336249
47	6	0	-5.486894	3.371110	-1.592143
48	6	0	-3.083523	-5.261974	-5.170559
49	9	0	-5.012818	-6.182603	-4.185654
50	9	0	-1.162594	-4.304432	-6.136800
51	1	0	-8.113223	5.199970	-2.757034
52	6	0	-6.400338	4.416483	-1.696403
53	1	0	-4.668974	3.437515	-0.882491
54	9	0	-2.446162	-6.416654	-5.025759
55	1	0	-6.295837	5.289283	-1.060162

TS3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.587990	-2.232589	-2.633065

2	6	0	-1.490022	-3.109746	-2.444798
3	6	0	-1.665816	-4.266396	-1.667446
4	6	0	-2.910168	-4.502895	-1.106574
5	6	0	-3.983212	-3.617620	-1.316965
6	6	0	-3.865645	-2.481387	-2.106152
7	1	0	-0.841881	-4.956332	-1.512248
8	1	0	-3.066561	-5.387838	-0.497360
9	1	0	-4.952127	-3.801711	-0.864882
10	6	0	-0.381157	-2.556657	-3.174329
11	1	0	0.615661	-2.965593	-3.249332
12	6	0	-0.824291	-1.405905	-3.761942
13	1	0	-0.307510	-0.701418	-4.397072
14	7	0	-2.146182	-1.200967	-3.431258
15	1	0	-2.725019	-0.465001	-3.802611
16	6	0	-5.107367	-1.604220	-2.274996
17	1	0	-4.632290	-0.310603	-2.317057
18	8	0	-5.909084	-1.573802	-1.239072
19	6	0	-5.644951	-1.558020	-3.618436
20	7	0	-6.778542	-0.882733	-4.077572
21	7	0	-4.940435	-1.869207	-4.773699
22	6	0	-6.585382	-0.742002	-5.459829
23	6	0	-8.249314	-0.909327	-3.725583
24	7	0	-5.527262	-1.316069	-5.901952
25	6	0	-4.113329	-2.990399	-4.979561
26	6	0	-7.480158	0.084805	-6.339180
27	6	0	-8.876967	0.251080	-4.530786
28	1	0	-8.624602	-1.854609	-4.142022
29	6	0	-8.910748	-0.716120	-2.361463
30	6	0	-4.419087	-4.229892	-4.424258
31	6	0	-2.924351	-2.850544	-5.689599
32	1	0	-7.414087	-0.286857	-7.361922
33	1	0	-7.119484	1.125212	-6.314399
34	8	0	-8.821687	0.025084	-5.917674
35	1	0	-8.309636	1.163385	-4.275679
36	6	0	-10.294198	0.377239	-4.010149
37	6	0	-10.102904	0.000260	-2.564934
38	6	0	-8.647862	-1.265819	-1.109657
39	6	0	-3.514323	-5.277863	-4.490476
40	9	0	-5.566001	-4.402616	-3.771576
41	6	0	-2.027490	-3.900897	-5.789006
42	9	0	-2.607938	-1.670204	-6.220393
43	1	0	-10.716268	1.372621	-4.161863
44	1	0	-10.935117	-0.350772	-4.523376
45	6	0	-10.986356	0.241310	-1.520258
46	1	0	-7.736978	-1.830839	-0.959106
47	6	0	-9.537661	-1.019127	-0.063253
48	6	0	-2.320593	-5.113817	-5.178868
49	9	0	-3.796178	-6.443233	-3.914902
50	9	0	-0.876651	-3.743009	-6.437583
51	1	0	-11.895852	0.808390	-1.696397
52	6	0	-10.691553	-0.262055	-0.255881
53	1	0	-9.323386	-1.429654	0.918888
54	9	0	-1.451081	-6.116688	-5.249051
55	1	0	-11.367015	-0.076145	0.573492
56	6	0	-3.738779	1.828700	-2.988596
57	1	0	-2.649362	1.757485	-3.059247
58	1	0	-3.960069	2.886272	-2.802463
59	6	0	-4.339498	1.431653	-4.337303
60	1	0	-5.423707	1.335047	-4.289672
61	1	0	-4.098987	2.209962	-5.066291
62	1	0	-3.947470	0.494021	-4.744291

63	6	0	-2.982078	0.780987	-0.913800
64	1	0	-2.226298	0.422312	-1.615472
65	6	0	-3.172522	-0.330453	0.134179
66	1	0	-4.071242	-0.922042	-0.052409
67	1	0	-2.310123	-1.002640	0.101475
68	1	0	-3.231877	0.082338	1.144737
69	6	0	-2.442815	2.063208	-0.276019
70	1	0	-1.493998	1.834870	0.216963
71	1	0	-2.257263	2.852033	-1.010889
72	1	0	-3.123969	2.451746	0.486241
73	6	0	-5.296252	1.774530	-1.106138
74	1	0	-4.914942	2.791076	-0.926689
75	6	0	-6.520113	1.869696	-2.012577
76	1	0	-7.341370	2.332763	-1.459680
77	1	0	-6.347723	2.471248	-2.907555
78	1	0	-6.829566	0.858364	-2.291320
79	6	0	-5.728619	1.177699	0.230219
80	1	0	-6.015787	0.132948	0.086870
81	1	0	-4.958031	1.254527	0.997190
82	1	0	-6.594260	1.747327	0.579900
83	7	0	-4.182844	1.029851	-1.800205

TS4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.608585	-2.279414	-2.599417
2	6	0	-1.521828	-3.153261	-2.343710
3	6	0	-1.750700	-4.347428	-1.641805
4	6	0	-3.038567	-4.635715	-1.225717
5	6	0	-4.105199	-3.761338	-1.502976
6	6	0	-3.926846	-2.574688	-2.206455
7	1	0	-0.931390	-5.028709	-1.435517
8	1	0	-3.239152	-5.553412	-0.683211
9	1	0	-5.107664	-4.018534	-1.178306
10	6	0	-0.354037	-2.558945	-2.932809
11	1	0	0.649733	-2.956423	-2.922953
12	6	0	-0.751789	-1.389848	-3.513196
13	1	0	-0.186238	-0.652559	-4.063723
14	7	0	-2.105203	-1.210956	-3.306787
15	1	0	-2.642988	-0.470462	-3.727077
16	6	0	-5.104980	-1.660691	-2.459893
17	1	0	-4.667388	-0.281586	-2.217805
18	8	0	-6.124458	-1.844353	-1.506526
19	6	0	-5.722915	-1.702558	-3.771842
20	7	0	-6.908130	-1.153845	-4.195448
21	7	0	-5.076741	-2.048135	-4.919469
22	6	0	-6.831252	-1.109904	-5.590350
23	6	0	-8.335026	-0.936104	-3.709519
24	7	0	-5.754205	-1.649093	-6.045050
25	6	0	-4.041274	-2.998370	-5.083550
26	6	0	-7.805122	-0.374867	-6.484310
27	6	0	-8.794718	0.303091	-4.515122
28	1	0	-8.863448	-1.814499	-4.097942
29	6	0	-8.857151	-0.657474	-2.306824
30	6	0	-4.208635	-4.297029	-4.613839
31	6	0	-2.851411	-2.641481	-5.704292
32	1	0	-8.014815	-0.983799	-7.364457
33	1	0	-7.294519	0.544397	-6.807301
34	8	0	-9.023591	-0.061866	-5.854122

35	1	0	-7.991876	1.056641	-4.464311
36	6	0	-10.025684	0.837800	-3.810610
37	6	0	-9.803396	0.376891	-2.392786
38	6	0	-8.761983	-1.391881	-1.124687
39	6	0	-3.165146	-5.205766	-4.679552
40	9	0	-5.353503	-4.643983	-4.038093
41	6	0	-1.808803	-3.548930	-5.796051
42	9	0	-2.681712	-1.394111	-6.137070
43	1	0	-10.136585	1.918241	-3.920398
44	1	0	-10.920820	0.357901	-4.223745
45	6	0	-10.516039	0.791914	-1.273165
46	1	0	-8.141099	-2.272971	-1.069842
47	6	0	-9.479203	-0.977794	-0.004586
48	6	0	-1.969436	-4.828770	-5.278440
49	9	0	-3.304129	-6.427961	-4.181597
50	9	0	-0.655354	-3.194128	-6.347724
51	1	0	-11.228195	1.607455	-1.353921
52	6	0	-10.326232	0.128749	-0.064852
53	1	0	-9.385359	-1.535245	0.921588
54	9	0	-0.964018	-5.688757	-5.336152
55	1	0	-10.870301	0.444259	0.819462
56	6	0	-3.831875	1.698437	-3.015712
57	1	0	-2.741742	1.642943	-3.064751
58	1	0	-4.070299	2.755891	-2.868656
59	6	0	-4.413485	1.233096	-4.352275
60	1	0	-5.498706	1.132415	-4.326940
61	1	0	-4.166271	1.983207	-5.106947
62	1	0	-4.003261	0.285675	-4.714555
63	6	0	-3.078259	0.758457	-0.877017
64	1	0	-2.297684	0.424898	-1.561869
65	6	0	-3.210406	-0.343678	0.182280
66	1	0	-3.911021	-1.130580	-0.099231
67	1	0	-2.236207	-0.827221	0.293163
68	1	0	-3.495375	0.045051	1.160686
69	6	0	-2.617008	2.068758	-0.243058
70	1	0	-1.659946	1.891109	0.253503
71	1	0	-2.468142	2.861210	-0.981474
72	1	0	-3.320003	2.422853	0.516124
73	6	0	-5.421600	1.703157	-1.152921
74	1	0	-5.019766	2.694696	-0.912158
75	6	0	-6.571473	1.867145	-2.140393
76	1	0	-7.440132	2.274159	-1.617705
77	1	0	-6.337870	2.534557	-2.971833
78	1	0	-6.855263	0.883669	-2.525130
79	6	0	-5.967357	1.079836	0.125736
80	1	0	-6.451020	0.121698	-0.080742
81	1	0	-5.226301	0.962289	0.912537
82	1	0	-6.744870	1.745536	0.508226
83	7	0	-4.281413	0.941074	-1.791032
84	1	0	-5.784610	-1.602808	-0.635104

TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.656340	-1.869879	-2.729061
2	6	0	-1.435365	-2.583605	-2.613364
3	6	0	-1.396145	-3.774647	-1.872260
4	6	0	-2.562950	-4.214487	-1.273280
5	6	0	-3.762791	-3.497700	-1.416186

6	6	0	-3.860140	-2.326002	-2.159248
7	1	0	-0.469387	-4.330892	-1.774536
8	1	0	-2.565031	-5.127565	-0.686418
9	1	0	-4.650981	-3.875308	-0.926110
10	6	0	-0.448222	-1.858271	-3.363736
11	1	0	0.592423	-2.118683	-3.485392
12	6	0	-1.074163	-0.769214	-3.895402
13	1	0	-0.692539	0.020063	-4.526095
14	7	0	-2.398290	-0.763282	-3.506123
15	1	0	-3.080663	-0.113972	-3.861386
16	6	0	-5.184108	-1.600201	-2.252716
17	1	0	-4.859937	-0.252652	-1.896544
18	8	0	-6.058959	-1.950979	-1.223945
19	6	0	-5.825313	-1.511901	-3.566086
20	7	0	-6.987731	-0.863764	-3.958597
21	7	0	-5.172770	-1.777282	-4.733491
22	6	0	-6.880635	-0.728631	-5.348570
23	6	0	-8.437744	-0.777877	-3.470873
24	7	0	-5.815837	-1.264440	-5.829666
25	6	0	-4.184864	-2.759569	-4.985576
26	6	0	-7.848697	0.017133	-6.222320
27	6	0	-9.115724	0.304888	-4.349031
28	1	0	-8.855428	-1.751656	-3.758056
29	6	0	-9.001972	-0.416338	-2.088040
30	6	0	-4.309171	-4.035788	-4.450858
31	6	0	-3.068880	-2.450208	-5.756056
32	1	0	-7.835723	-0.430020	-7.216254
33	1	0	-7.510943	1.061783	-6.294686
34	8	0	-9.150373	-0.048978	-5.704173
35	1	0	-8.549513	1.243141	-4.212881
36	6	0	-10.502142	0.461471	-3.762400
37	6	0	-10.215458	0.261519	-2.302201
38	6	0	-8.642063	-0.741191	-0.783731
39	6	0	-3.290023	-4.962974	-4.586528
40	9	0	-5.389234	-4.346975	-3.734281
41	6	0	-2.054173	-3.379116	-5.921459
42	9	0	-2.935053	-1.232894	-6.271349
43	1	0	-10.953114	1.426296	-3.999975
44	1	0	-11.151297	-0.331563	-4.153866
45	6	0	-11.028078	0.649007	-1.244545
46	1	0	-7.722697	-1.264317	-0.585658
47	6	0	-9.456561	-0.348475	0.278699
48	6	0	-2.163782	-4.632304	-5.329173
49	9	0	-3.392058	-6.156039	-4.014977
50	9	0	-0.969172	-3.067654	-6.618736
51	1	0	-11.953725	1.180830	-1.442197
52	6	0	-10.641469	0.348076	0.058143
53	1	0	-9.149435	-0.592502	1.291435
54	9	0	-1.180690	-5.509985	-5.461421
55	1	0	-11.262146	0.650001	0.895267
56	6	0	-4.064776	1.884859	-2.486391
57	1	0	-2.991743	1.768269	-2.656665
58	1	0	-4.209060	2.920773	-2.159943
59	6	0	-4.788946	1.684869	-3.819288
60	1	0	-5.864861	1.834142	-3.751720
61	1	0	-4.392878	2.417444	-4.526565
62	1	0	-4.631710	0.699526	-4.268706
63	6	0	-3.186868	0.657036	-0.557297
64	1	0	-2.470461	0.376662	-1.331934
65	6	0	-3.306027	-0.546522	0.393828
66	1	0	-4.158450	-1.185435	0.162524

67	1	0	-2.404090	-1.157871	0.299339
68	1	0	-3.384764	-0.230004	1.436017
69	6	0	-2.628349	1.876576	0.173262
70	1	0	-1.653218	1.608854	0.588052
71	1	0	-2.485678	2.736224	-0.486876
72	1	0	-3.267182	2.175760	1.008859
73	6	0	-5.526874	1.626807	-0.531849
74	1	0	-5.105920	2.576580	-0.175649
75	6	0	-6.735721	1.958202	-1.405637
76	1	0	-7.593305	2.192764	-0.771037
77	1	0	-6.555856	2.817984	-2.053513
78	1	0	-7.010866	1.099186	-2.021749
79	6	0	-5.941028	0.805157	0.685226
80	1	0	-6.164965	-0.228435	0.413355
81	1	0	-5.176245	0.806630	1.461374
82	1	0	-6.843137	1.251625	1.110053
83	7	0	-4.443691	0.970468	-1.354090
84	6	0	-8.059034	-4.213441	-2.099409
85	1	0	-7.522242	-4.664507	-2.939060
86	6	0	-7.981122	-4.092460	0.361788
87	1	0	-8.636608	-3.275312	0.036741
88	6	0	-7.057732	-3.486728	1.428391
89	1	0	-6.320754	-2.812761	0.982569
90	1	0	-7.663676	-2.911087	2.135424
91	1	0	-6.528383	-4.249730	2.002867
92	6	0	-8.884854	-5.154038	1.003412
93	1	0	-9.451768	-4.687402	1.814889
94	1	0	-9.597188	-5.581041	0.296585
95	1	0	-8.303680	-5.970002	1.440824
96	6	0	-6.523573	-5.764825	-0.953956
97	6	0	-5.653885	-6.037752	0.273579
98	1	0	-6.246989	-6.346367	1.137888
99	1	0	-5.053396	-5.173776	0.566138
100	1	0	-4.972346	-6.859252	0.036624
101	7	0	-7.264427	-4.478311	-0.882261
102	1	0	-6.289284	-2.934207	-1.204593
103	1	0	-8.034374	-3.126697	-2.262839
104	6	0	-9.530591	-4.635135	-2.148341
105	1	0	-9.930465	-4.383824	-3.135699
106	1	0	-9.672596	-5.706260	-1.992085
107	1	0	-10.128090	-4.095541	-1.408381
108	6	0	-7.366504	-7.006778	-1.276652
109	1	0	-6.706520	-7.877074	-1.341160
110	1	0	-8.114646	-7.209004	-0.506550
111	1	0	-7.873285	-6.911290	-2.239632
112	1	0	-5.835936	-5.631154	-1.800395

TS6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-16.089317	-2.657024	26.896619
2	6	0	-16.195318	-3.934886	27.491259
3	6	0	-16.893398	-4.079475	28.700733
4	6	0	-17.465189	-2.949641	29.275174
5	6	0	-17.362373	-1.693365	28.669106
6	6	0	-16.615478	-1.488964	27.497999
7	1	0	-16.995340	-5.055670	29.166520
8	1	0	-18.016467	-3.041038	30.206307
9	1	0	-17.798127	-0.821340	29.146198

10	6	0	-15.535340	-4.860553	26.613822
11	1	0	-15.423606	-5.924684	26.761566
12	6	0	-15.069864	-4.139082	25.550665
13	1	0	-14.516723	-4.454120	24.678049
14	7	0	-15.398201	-2.810152	25.720424
15	1	0	-15.176294	-2.079849	25.061723
16	6	0	-16.369008	-0.130574	27.025168
17	8	0	-17.275299	0.799286	27.078952
18	6	0	-15.034448	0.277670	26.702543
19	7	0	-14.575275	1.433554	26.103840
20	7	0	-13.873944	-0.409239	27.006066
21	6	0	-13.195859	1.346582	26.080439
22	6	0	-15.020241	2.805327	25.693682
23	7	0	-12.747294	0.257908	26.608789
24	6	0	-13.691723	-1.476943	27.911592
25	6	0	-12.361310	2.471403	25.549469
26	6	0	-14.111377	3.739271	26.531186
27	1	0	-14.732509	2.871587	24.636027
28	6	0	-16.384036	3.436631	25.845181
29	6	0	-13.008786	-2.618884	27.504754
30	6	0	-14.205156	-1.416003	29.204550
31	1	0	-12.428164	2.484284	24.454394
32	1	0	-11.322955	2.293392	25.832772
33	8	0	-12.775893	3.728788	26.071319
34	1	0	-14.154839	3.364222	27.565069
35	6	0	-14.763880	5.112230	26.473257
36	6	0	-16.219692	4.753281	26.293491
37	6	0	-17.622876	3.002480	25.391938
38	6	0	-12.893947	-3.709664	28.351510
39	9	0	-12.509421	-2.689898	26.275723
40	6	0	-14.118958	-2.512777	30.046522
41	9	0	-14.825832	-0.317584	29.621737
42	1	0	-14.556994	5.715543	27.359333
43	1	0	-14.396296	5.654769	25.594266
44	6	0	-17.319331	5.597687	26.414326
45	1	0	-17.739907	2.021889	24.956671
46	6	0	-18.723411	3.844403	25.516874
47	6	0	-13.458781	-3.657394	29.619000
48	9	0	-12.273983	-4.812011	27.944748
49	9	0	-14.655556	-2.469304	31.260564
50	1	0	-17.191024	6.612615	26.778072
51	6	0	-18.577349	5.128731	26.046112
52	1	0	-19.698250	3.494908	25.191725
53	9	0	-13.374050	-4.708655	30.423547
54	1	0	-19.444151	5.774639	26.143361
55	6	0	-20.232524	-1.157688	26.885015
56	6	0	-20.255830	-2.457745	27.324781
57	6	0	-19.510458	-3.503222	26.698673
58	6	0	-18.868410	-3.177597	25.468301
59	6	0	-18.831351	-1.897255	24.964217
60	6	0	-19.384603	-0.850975	25.770768
61	1	0	-20.873553	-2.705544	28.175897
62	1	0	-18.357179	-3.961104	24.925328
63	6	0	-19.429792	-4.803996	27.277404
64	6	0	-18.810082	-5.901010	26.594930
65	6	0	-19.961666	-5.080741	28.581064
66	6	0	-18.739729	-7.164157	27.102185
67	1	0	-18.381430	-5.716690	25.619176
68	6	0	-19.927086	-6.309156	29.169306
69	1	0	-20.382915	-4.255838	29.139107
70	6	0	-19.323016	-7.439930	28.434221

71	6	0	-21.089005	-0.059928	27.534296
72	6	0	-21.978521	0.575864	26.449565
73	1	0	-22.596036	1.365262	26.891835
74	1	0	-21.370911	1.015001	25.655465
75	1	0	-22.645903	-0.172502	26.009746
76	6	0	-22.008376	-0.642647	28.615556
77	1	0	-21.436511	-1.054796	29.454088
78	1	0	-22.647010	0.153672	29.008431
79	1	0	-22.658433	-1.428594	28.218069
80	6	0	-20.239599	1.040459	28.198260
81	1	0	-19.685394	1.629033	27.467140
82	1	0	-20.902878	1.714984	28.751529
83	1	0	-19.524966	0.612064	28.907030
84	6	0	-18.268055	-1.582971	23.571845
85	6	0	-19.430823	-1.045463	22.713785
86	1	0	-20.221326	-1.796098	22.617327
87	1	0	-19.855517	-0.143517	23.163298
88	1	0	-19.070518	-0.794475	21.709971
89	6	0	-17.724026	-2.846392	22.892971
90	1	0	-17.382834	-2.593926	21.884939
91	1	0	-16.876644	-3.269096	23.443859
92	1	0	-18.493142	-3.619183	22.800498
93	6	0	-17.148920	-0.520869	23.576713
94	1	0	-16.466707	-0.652697	24.422135
95	1	0	-16.570175	-0.588605	22.649549
96	1	0	-17.563254	0.483661	23.647534
97	6	0	-20.474736	-6.551134	30.576958
98	6	0	-21.035129	-5.267312	31.200144
99	1	0	-21.413501	-5.491480	32.202023
100	1	0	-20.266010	-4.493633	31.299442
101	1	0	-21.864807	-4.858214	30.613957
102	6	0	-19.346138	-7.060778	31.493266
103	1	0	-18.542240	-6.318532	31.555822
104	1	0	-19.735812	-7.223313	32.504318
105	1	0	-18.932906	-7.997623	31.119266
106	6	0	-21.616029	-7.583978	30.528432
107	1	0	-22.433599	-7.218352	29.898169
108	1	0	-21.263755	-8.535537	30.131259
109	1	0	-22.012330	-7.744831	31.537272
110	6	0	-18.084442	-8.312427	26.331944
111	6	0	-17.530287	-7.849111	24.979093
112	1	0	-16.779846	-7.059428	25.093565
113	1	0	-17.053972	-8.697237	24.478278
114	1	0	-18.323483	-7.476394	24.322228
115	6	0	-19.120288	-9.419082	26.056788
116	1	0	-19.511774	-9.827252	26.988134
117	1	0	-19.952784	-9.022824	25.465839
118	1	0	-18.652363	-10.227549	25.483944
119	6	0	-16.913371	-8.891705	27.147835
120	1	0	-16.154152	-8.123330	27.330652
121	1	0	-17.259274	-9.276240	28.107241
122	1	0	-16.439869	-9.706321	26.588736
123	8	0	-19.064462	0.401279	25.529328
124	8	0	-19.296666	-8.582976	28.921314
125	1	0	-18.222975	0.640970	26.300136

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-16.914070	-2.527495	27.257299
2	6	0	-15.720622	-3.158309	26.782199
3	6	0	-14.733019	-2.404647	26.144914
4	6	0	-14.916790	-1.033650	25.968962
5	6	0	-16.109092	-0.426713	26.357038
6	6	0	-17.145237	-1.159908	26.962474
7	1	0	-13.832039	-2.886242	25.775298
8	1	0	-14.153440	-0.443537	25.474971
9	1	0	-16.295487	0.614987	26.118402
10	6	0	-15.860269	-4.550690	27.091911
11	1	0	-15.156668	-5.341233	26.875166
12	6	0	-17.064359	-4.667984	27.728807
13	1	0	-17.518432	-5.561802	28.141850
14	7	0	-17.722220	-3.452961	27.855435
15	1	0	-18.293687	-3.384644	28.997543
16	6	0	-18.449001	-0.499656	26.938247
17	8	0	-18.640857	0.698792	26.874882
18	6	0	-19.709321	-1.328212	26.698307
19	7	0	-20.968323	-1.093935	27.121961
20	7	0	-19.814880	-2.257902	25.743200
21	6	0	-21.779626	-1.958932	26.405464
22	6	0	-21.618599	-0.328853	28.238449
23	7	0	-21.092495	-2.662549	25.556654
24	6	0	-18.783376	-2.810028	24.938900
25	6	0	-23.279647	-2.036461	26.541651
26	6	0	-23.071568	-0.102215	27.777919
27	1	0	-21.658317	-1.045847	29.068957
28	6	0	-21.230690	1.032160	28.798861
29	6	0	-18.540406	-4.177315	24.992881
30	6	0	-17.985990	-1.987157	24.150386
31	1	0	-23.572466	-3.083047	26.641162
32	1	0	-23.716636	-1.630391	25.619371
33	8	0	-23.738092	-1.335510	27.671974
34	1	0	-23.048218	0.410300	26.803308
35	6	0	-23.644320	0.827517	28.829845
36	6	0	-22.432841	1.660036	29.171872
37	6	0	-20.015582	1.605766	29.163955
38	6	0	-17.471359	-4.716378	24.294585
39	9	0	-19.292621	-4.959562	25.753514
40	6	0	-16.904364	-2.518329	23.467894
41	9	0	-18.226046	-0.681074	24.101278
42	1	0	-24.493799	1.407357	28.466589
43	1	0	-23.969374	0.239482	29.696833
44	6	0	-22.425884	2.881124	29.832854
45	1	0	-19.069358	1.140779	28.934903
46	6	0	-20.013987	2.832229	29.827524
47	6	0	-16.654106	-3.884054	23.539870
48	9	0	-17.206006	-6.011878	24.378054
49	9	0	-16.110685	-1.732444	22.754653
50	1	0	-23.363038	3.359404	30.100112
51	6	0	-21.207071	3.473958	30.150882
52	1	0	-19.065290	3.286116	30.093117
53	9	0	-15.611476	-4.391436	22.903182
54	1	0	-21.186104	4.430434	30.662501
55	6	0	-19.978326	-4.427937	29.924001
56	1	0	-20.564420	-4.566167	30.837436

57	1	0	-19.516403	-5.387725	29.688238
58	6	0	-20.884023	-4.039265	28.762464
59	1	0	-20.297376	-3.859331	27.857279
60	1	0	-21.560854	-4.871759	28.558267
61	1	0	-21.509589	-3.168901	28.985845
62	6	0	-19.362957	-2.069574	30.392256
63	1	0	-19.813344	-1.799620	29.428574
64	6	0	-18.233291	-1.073039	30.641890
65	1	0	-18.674677	-0.082232	30.763700
66	1	0	-17.678440	-1.292630	31.556573
67	1	0	-17.529874	-1.034452	29.804146
68	6	0	-20.434588	-1.964774	31.474966
69	1	0	-20.754335	-0.921568	31.555297
70	1	0	-21.318205	-2.568518	31.255305
71	1	0	-20.045866	-2.267255	32.451943
72	6	0	-17.891962	-3.915089	31.244210
73	1	0	-18.119616	-3.313602	32.130278
74	6	0	-18.030288	-5.379581	31.656788
75	1	0	-17.301190	-5.563099	32.449457
76	1	0	-19.017136	-5.625600	32.051063
77	1	0	-17.792045	-6.058703	30.832926
78	6	0	-16.441233	-3.662318	30.821140
79	1	0	-16.289361	-2.688739	30.355205
80	1	0	-15.801503	-3.719499	31.705536
81	1	0	-16.108907	-4.425809	30.112905
82	7	0	-18.862635	-3.467108	30.166395

***Re*-TS8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-19.512330	-1.615182	26.336878
2	6	0	-18.783383	-2.464801	27.236789
3	6	0	-17.428996	-2.723052	27.002110
4	6	0	-16.803771	-2.204101	25.870139
5	6	0	-17.507521	-1.387541	24.978943
6	6	0	-18.841396	-1.059892	25.223855
7	1	0	-16.864858	-3.352531	27.686464
8	1	0	-15.759914	-2.428482	25.677340
9	1	0	-17.002995	-0.963970	24.112301
10	6	0	-19.744830	-2.892193	28.200257
11	1	0	-19.584375	-3.545385	29.046808
12	6	0	-20.935322	-2.315544	27.805985
13	1	0	-21.902859	-2.436323	28.278938
14	7	0	-20.821247	-1.527980	26.685985
15	6	0	-19.488193	-0.010343	24.460853
16	8	0	-20.108813	0.912131	24.946530
17	6	0	-19.402300	0.039580	22.928163
18	7	0	-19.375826	-0.880474	21.944853
19	7	0	-19.552009	1.217791	22.302558
20	6	0	-19.549815	-0.188795	20.764514
21	6	0	-19.475042	-2.383622	21.816252
22	7	0	-19.636966	1.090817	20.956349
23	6	0	-19.655826	2.517885	22.861133
24	6	0	-19.559482	-0.928895	19.470290
25	6	0	-18.638604	-2.807249	20.555955
26	1	0	-20.546778	-2.553141	21.690148
27	6	0	-18.879959	-3.290056	22.864129
28	6	0	-18.652762	3.026960	23.675405
29	6	0	-20.785856	3.277598	22.595972

30	1	0	-19.378336	-0.235173	18.649785
31	1	0	-20.527305	-1.425074	19.315535
32	8	0	-18.494241	-1.846330	19.530857
33	1	0	-19.147178	-3.697422	20.162477
34	6	0	-17.264512	-3.188841	21.108629
35	6	0	-17.636954	-3.772097	22.442955
36	6	0	-19.495423	-3.789028	24.007169
37	6	0	-18.782465	4.286255	24.236127
38	9	0	-17.596818	2.273375	23.959118
39	6	0	-20.924773	4.538812	23.156089
40	9	0	-21.757176	2.790399	21.833443
41	1	0	-16.734821	-3.884864	20.455145
42	1	0	-16.655110	-2.282177	21.210038
43	6	0	-16.964736	-4.730267	23.190756
44	1	0	-20.472170	-3.429716	24.308808
45	6	0	-18.817765	-4.747622	24.755146
46	6	0	-19.920445	5.041942	23.971438
47	9	0	-17.831548	4.773712	25.021641
48	9	0	-22.021480	5.250197	22.924691
49	1	0	-16.004323	-5.113866	22.860402
50	6	0	-17.561232	-5.207071	24.355904
51	1	0	-19.272826	-5.131443	25.662567
52	9	0	-20.046909	6.245231	24.508909
53	1	0	-17.050449	-5.957396	24.951720
54	6	0	-22.268689	-1.218020	24.936826
55	8	0	-21.604451	-1.454278	23.930518
56	6	0	-23.112780	-2.391845	25.462259
57	9	0	-24.168541	-2.515186	24.632917
58	9	0	-22.454303	-3.550063	25.436091
59	9	0	-23.610504	-2.219948	26.691141
60	6	0	-22.770116	0.159628	25.249837
61	6	0	-22.920540	1.031750	24.168543
62	6	0	-23.102873	0.586535	26.536954
63	6	0	-23.409730	2.318852	24.368844
64	1	0	-22.640393	0.690385	23.175853
65	6	0	-23.584823	1.876085	26.735218
66	1	0	-22.940628	-0.077384	27.376944
67	6	0	-23.742202	2.741737	25.654054
68	1	0	-23.527022	2.994009	23.526834
69	1	0	-23.829338	2.210129	27.738233
70	1	0	-24.119578	3.747005	25.813285

***Si*-TS8**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-11.660236	-2.135346	26.002168
2	6	0	-11.369831	-2.315295	27.399006
3	6	0	-10.849817	-1.253757	28.148113
4	6	0	-10.636974	-0.019170	27.540980
5	6	0	-10.907254	0.162338	26.179234
6	6	0	-11.373383	-0.893653	25.391680
7	1	0	-10.607222	-1.392126	29.198776
8	1	0	-10.237614	0.808020	28.117999
9	1	0	-10.696008	1.114585	25.702301
10	6	0	-11.704835	-3.675246	27.675636
11	1	0	-11.628163	-4.189868	28.623293
12	6	0	-12.164573	-4.189858	26.481580
13	1	0	-12.527666	-5.195075	26.294916
14	7	0	-12.138804	-3.282801	25.453084

15	6	0	-11.431538	-0.645800	23.942840
16	8	0	-11.942310	0.322152	23.422787
17	6	0	-10.742975	-1.624016	23.000175
18	7	0	-10.975781	-1.719532	21.681115
19	7	0	-9.942647	-2.651120	23.298844
20	6	0	-10.455814	-2.928000	21.283322
21	6	0	-11.896905	-0.975687	20.806254
22	7	0	-9.774388	-3.487120	22.243929
23	6	0	-9.238814	-2.871616	24.507161
24	6	0	-10.789236	-3.567439	19.957399
25	6	0	-11.792410	-1.605816	19.407218
26	1	0	-12.893670	-1.147341	21.231579
27	6	0	-11.716745	0.479753	20.410447
28	6	0	-9.311513	-4.101169	25.152157
29	6	0	-8.542277	-1.817659	25.092484
30	1	0	-10.966031	-4.629380	20.132168
31	1	0	-9.952513	-3.450157	19.256537
32	8	0	-11.971846	-2.996959	19.433341
33	1	0	-10.780712	-1.386138	19.028446
34	6	0	-12.764561	-0.744181	18.611804
35	6	0	-12.330061	0.608630	19.149568
36	6	0	-11.097365	1.566897	21.009103
37	6	0	-8.735553	-4.255742	26.404016
38	9	0	-9.951123	-5.120403	24.602133
39	6	0	-7.976384	-1.965390	26.346583
40	9	0	-8.468388	-0.643807	24.468612
41	1	0	-12.642586	-0.838414	17.531921
42	1	0	-13.799453	-0.989627	18.878229
43	6	0	-12.382420	1.841052	18.515669
44	1	0	-10.592796	1.469404	21.961238
45	6	0	-11.140101	2.801179	20.357575
46	6	0	-8.078218	-3.187499	26.999529
47	9	0	-8.823465	-5.417579	27.038653
48	9	0	-7.341591	-0.951136	26.921505
49	1	0	-12.852239	1.938671	17.541704
50	6	0	-11.791781	2.943681	19.134762
51	1	0	-10.658335	3.659305	20.814430
52	9	0	-7.549553	-3.330324	28.206049
53	1	0	-11.819987	3.913356	18.648382
54	6	0	-14.730513	-5.626389	24.511446
55	6	0	-13.654900	-4.982232	23.897307
56	6	0	-12.616256	-5.733514	23.343229
57	6	0	-12.639626	-7.119599	23.419071
58	6	0	-13.714186	-7.764678	24.033501
59	6	0	-14.758747	-7.018459	24.571455
60	1	0	-15.546099	-5.056098	24.941657
61	1	0	-11.784616	-5.210441	22.882634
62	1	0	-11.822618	-7.699600	23.002010
63	1	0	-13.735045	-8.848158	24.092639
64	1	0	-15.597372	-7.518213	25.044767
65	6	0	-13.559066	-3.496751	23.769827
66	8	0	-13.028825	-2.967137	22.798302
67	6	0	-14.595634	-2.635196	24.517105
68	9	0	-14.237150	-1.351369	24.510109
69	9	0	-15.765255	-2.732806	23.850284
70	9	0	-14.841863	-2.995302	25.779151

***Re*-TS9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-18.950359	-1.344691	25.909752
2	6	0	-18.143711	-2.117123	26.761596
3	6	0	-16.751778	-1.957071	26.639158
4	6	0	-16.261338	-1.040095	25.715907
5	6	0	-17.110056	-0.274623	24.888541
6	6	0	-18.483241	-0.431599	24.968954
7	1	0	-16.068301	-2.537916	27.250211
8	1	0	-15.188382	-0.913878	25.617052
9	1	0	-16.690356	0.422281	24.168849
10	6	0	-19.059759	-2.898501	27.555515
11	1	0	-18.810476	-3.635089	28.305049
12	6	0	-20.330959	-2.550572	27.180184
13	1	0	-21.283305	-2.904190	27.546301
14	7	0	-20.268737	-1.613693	26.159418
15	6	0	-19.516059	0.293977	24.148555
16	8	0	-19.471539	1.495713	23.934035
17	6	0	-19.088235	-0.585706	22.332200
18	7	0	-18.780456	0.133562	21.228485
19	7	0	-18.442146	-1.738838	22.100567
20	6	0	-17.947731	-0.606091	20.421805
21	6	0	-19.264593	1.489711	20.901890
22	7	0	-17.720562	-1.778636	20.932471
23	6	0	-18.475441	-2.839378	22.980721
24	6	0	-17.387120	-0.039756	19.154240
25	6	0	-18.756987	1.873472	19.484077
26	1	0	-18.899387	2.153349	21.687033
27	6	0	-20.766435	1.525764	20.732940
28	6	0	-19.705404	-3.369119	23.360520
29	6	0	-17.307858	-3.327477	23.557070
30	1	0	-17.904743	-0.465264	18.286125
31	1	0	-16.330083	-0.299245	19.078262
32	8	0	-17.470652	1.368888	19.183628
33	1	0	-18.644293	2.959577	19.471729
34	6	0	-19.885161	1.479964	18.505103
35	6	0	-21.111004	1.528195	19.379679
36	6	0	-21.739004	1.551174	21.726473
37	6	0	-19.772697	-4.345984	24.342997
38	9	0	-20.818845	-2.938132	22.785741
39	6	0	-17.367921	-4.323418	24.518547
40	9	0	-16.132170	-2.813938	23.218148
41	1	0	-19.930238	2.158852	17.650671
42	1	0	-19.744995	0.468462	18.107377
43	6	0	-22.448930	1.558460	19.000059
44	1	0	-21.443140	1.557613	22.769719
45	6	0	-23.078603	1.571225	21.342415
46	6	0	-18.601839	-4.817954	24.921007
47	9	0	-20.946069	-4.832201	24.733325
48	9	0	-16.257699	-4.755475	25.108763
49	1	0	-22.725570	1.568047	17.949962
50	6	0	-23.429512	1.576141	19.990864
51	1	0	-23.855269	1.587718	22.100887
52	9	0	-18.662710	-5.737721	25.875335
53	1	0	-24.477347	1.598087	19.708054
54	6	0	-21.218683	-0.659519	25.603253
55	8	0	-20.812520	-0.346620	24.292853
56	6	0	-22.572544	-1.368608	25.430129

57	9	0	-23.430045	-0.608840	24.749775
58	9	0	-22.438244	-2.528208	24.788302
59	9	0	-23.109457	-1.629781	26.631905
60	6	0	-21.374149	0.585935	26.474165
61	6	0	-20.897665	0.628693	27.782874
62	6	0	-22.016867	1.701601	25.931790
63	6	0	-21.068132	1.781419	28.547192
64	1	0	-20.385697	-0.228766	28.209023
65	6	0	-22.188699	2.847651	26.698287
66	1	0	-22.370469	1.667630	24.907045
67	6	0	-21.714606	2.889384	28.008779
68	1	0	-20.689780	1.811390	29.563570
69	1	0	-22.684788	3.712166	26.269764
70	1	0	-21.843966	3.786920	28.605037

***Si*-TS9**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-18.799563	-1.333888	25.863699
2	6	0	-18.126301	-2.211233	26.727737
3	6	0	-16.724699	-2.103739	26.782397
4	6	0	-16.092507	-1.142508	26.001790
5	6	0	-16.811296	-0.279770	25.147511
6	6	0	-18.189272	-0.378097	25.066709
7	1	0	-16.140325	-2.763686	27.416407
8	1	0	-15.011701	-1.056859	26.041189
9	1	0	-16.292366	0.454878	24.539812
10	6	0	-19.154379	-3.028457	27.324123
11	1	0	-19.019116	-3.839790	28.024391
12	6	0	-20.355206	-2.611251	26.818792
13	1	0	-21.351098	-2.981165	27.011977
14	7	0	-20.147091	-1.587879	25.902986
15	6	0	-19.066755	0.434536	24.160880
16	8	0	-18.790896	1.592756	23.851635
17	6	0	-18.833577	-0.586527	22.496625
18	7	0	-18.759152	0.038815	21.297995
19	7	0	-18.214853	-1.751308	22.255081
20	6	0	-18.075002	-0.769617	20.417775
21	6	0	-19.302356	1.371079	20.926155
22	7	0	-17.731305	-1.889193	20.976262
23	6	0	-18.086440	-2.834324	23.153760
24	6	0	-17.796092	-0.366055	19.001962
25	6	0	-19.249786	1.462887	19.381366
26	1	0	-18.702110	2.122100	21.439128
27	6	0	-20.789681	1.483493	21.174603
28	6	0	-19.218895	-3.496394	23.618892
29	6	0	-16.829248	-3.255942	23.568073
30	1	0	-18.401009	-0.975140	18.318847
31	1	0	-16.743756	-0.546546	18.776024
32	8	0	-18.034245	1.011259	18.825895
33	1	0	-19.310715	2.522877	19.124322
34	6	0	-20.541675	0.761499	18.904557
35	6	0	-21.492491	1.103544	20.024485
36	6	0	-21.455116	1.954497	22.300563
37	6	0	-19.098722	-4.561987	24.495920
38	9	0	-20.427550	-3.099554	23.237471
39	6	0	-16.701376	-4.324912	24.442327
40	9	0	-15.743623	-2.616029	23.155092
41	1	0	-20.869584	1.123301	17.927801

42	1	0	-20.408880	-0.324457	18.827427
43	6	0	-22.882032	1.128286	20.011924
44	1	0	-20.893481	2.265743	23.172465
45	6	0	-22.849394	1.977674	22.284137
46	6	0	-17.837279	-4.972761	24.906191
47	9	0	-20.181227	-5.172758	24.964786
48	9	0	-15.501371	-4.691490	24.880641
49	1	0	-23.433378	0.837912	19.122610
50	6	0	-23.555514	1.556158	21.156980
51	1	0	-23.389040	2.322597	23.160586
52	9	0	-17.721859	-5.960003	25.785002
53	1	0	-24.640920	1.578381	21.163805
54	6	0	-21.054174	-0.561647	25.398635
55	8	0	-20.478522	0.144355	24.339453
56	6	0	-21.272337	0.483056	26.521251
57	9	0	-22.187913	1.382412	26.159057
58	9	0	-20.132788	1.134030	26.782098
59	9	0	-21.674165	-0.083224	27.670081
60	6	0	-22.379649	-1.144880	24.915471
61	6	0	-23.348528	-1.608004	25.810989
62	6	0	-22.620091	-1.217928	23.542738
63	6	0	-24.537260	-2.153373	25.332949
64	1	0	-23.194929	-1.534750	26.881581
65	6	0	-23.813014	-1.757858	23.071501
66	1	0	-21.874995	-0.839412	22.851656
67	6	0	-24.772677	-2.230009	23.963057
68	1	0	-25.281534	-2.510896	26.036695
69	1	0	-23.992707	-1.799519	22.001916
70	1	0	-25.702850	-2.648752	23.592752

***Si*-INT1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.597724	0.584435	-1.031536
2	6	0	-3.241815	1.710113	-0.247879
3	6	0	-4.215396	2.301273	0.576889
4	6	0	-5.489475	1.759437	0.598570
5	6	0	-5.825216	0.656318	-0.212458
6	6	0	-4.898322	0.058010	-1.047096
7	1	0	-3.967847	3.168939	1.181026
8	1	0	-6.252141	2.203862	1.231437
9	1	0	-6.831760	0.249795	-0.234589
10	6	0	-1.862075	1.994417	-0.528883
11	1	0	-1.263533	2.788933	-0.108560
12	6	0	-1.441585	1.064656	-1.436134
13	1	0	-0.472274	0.927004	-1.892385
14	7	0	-2.482187	0.219174	-1.752732
15	1	0	-2.386242	-0.605837	-2.322111
16	6	0	-5.343402	-1.087689	-1.966697
17	1	0	-4.615428	-1.928575	-1.792797
18	8	0	-6.631115	-1.410582	-1.917990
19	6	0	-5.065750	-0.698383	-3.437196
20	7	0	-4.673871	-1.497419	-4.445718
21	7	0	-5.357623	0.463523	-4.029062
22	6	0	-4.671918	-0.739573	-5.603081
23	6	0	-4.116365	-2.855452	-4.444169
24	7	0	-5.106721	0.460898	-5.374199
25	6	0	-5.910034	1.596321	-3.384281
26	6	0	-4.160549	-1.275409	-6.918660

27	6	0	-4.060569	-3.324281	-5.903819
28	1	0	-3.087134	-2.771220	-4.071309
29	6	0	-4.785705	-4.059887	-3.811442
30	6	0	-5.074899	2.611291	-2.929355
31	6	0	-7.270391	1.629026	-3.103910
32	1	0	-3.553668	-0.508550	-7.400776
33	1	0	-5.012516	-1.518004	-7.567396
34	8	0	-3.350413	-2.417989	-6.710363
35	1	0	-5.099012	-3.397485	-6.265356
36	6	0	-3.513677	-4.739165	-5.752228
37	6	0	-4.327437	-5.171599	-4.544087
38	6	0	-5.657375	-4.206857	-2.740614
39	6	0	-5.590713	3.646669	-2.169381
40	9	0	-3.776392	2.566679	-3.191528
41	6	0	-7.794418	2.674405	-2.357386
42	9	0	-8.069019	0.675207	-3.550417
43	1	0	-3.678652	-5.363555	-6.631484
44	1	0	-2.438109	-4.705914	-5.538244
45	6	0	-4.696152	-6.454429	-4.168581
46	1	0	-6.095406	-3.340807	-2.239210
47	6	0	-6.026354	-5.506944	-2.379697
48	6	0	-6.950597	3.669758	-1.883253
49	9	0	-4.796239	4.599667	-1.696660
50	9	0	-9.094207	2.722826	-2.084521
51	1	0	-4.352345	-7.315104	-4.734406
52	6	0	-5.541155	-6.615901	-3.068720
53	1	0	-6.713706	-5.650200	-1.552008
54	9	0	-7.446449	4.655789	-1.149407
55	1	0	-5.843491	-7.613326	-2.765867

***Re*-INT1**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.101528	-2.175192	-2.764785
2	6	0	-2.279374	-3.283057	-2.446143
3	6	0	-2.831802	-4.349027	-1.711871
4	6	0	-4.161077	-4.279325	-1.331455
5	6	0	-4.963447	-3.174293	-1.684385
6	6	0	-4.461064	-2.117868	-2.420532
7	1	0	-2.224207	-5.211995	-1.455686
8	1	0	-4.600444	-5.093119	-0.763027
9	1	0	-6.010648	-3.119195	-1.406615
10	6	0	-0.991192	-3.026673	-3.029881
11	1	0	-0.119656	-3.663429	-2.990403
12	6	0	-1.073012	-1.815874	-3.659549
13	1	0	-0.324516	-1.266013	-4.210845
14	7	0	-2.341568	-1.299201	-3.507336
15	1	0	-2.631927	-0.391667	-3.836767
16	6	0	-5.380012	-0.958590	-2.812960
17	1	0	-4.760917	-0.028437	-2.660798
18	8	0	-6.583481	-0.944891	-2.253579
19	6	0	-5.632978	-0.918395	-4.341084
20	7	0	-6.388040	0.036289	-4.921951
21	7	0	-5.367329	-1.783486	-5.329023
22	6	0	-6.552628	-0.318007	-6.246832
23	6	0	-7.181884	1.186181	-4.406761
24	7	0	-5.934789	-1.423448	-6.522067
25	6	0	-4.577094	-2.960096	-5.292138
26	6	0	-7.303185	0.513121	-7.258290

27	6	0	-7.286181	2.130522	-5.620518
28	1	0	-8.167756	0.769282	-4.171239
29	6	0	-6.760476	2.150397	-3.307287
30	6	0	-5.056527	-4.115049	-4.688004
31	6	0	-3.303968	-2.942474	-5.848765
32	1	0	-7.991461	-0.128337	-7.810593
33	1	0	-6.568348	0.929156	-7.961284
34	8	0	-8.047763	1.543550	-6.647642
35	1	0	-6.258947	2.316032	-5.976669
36	6	0	-7.831331	3.427795	-5.058652
37	6	0	-7.150868	3.440072	-3.709285
38	6	0	-6.286191	1.937823	-2.014467
39	6	0	-4.244444	-5.234516	-4.592190
40	9	0	-6.274487	-4.134901	-4.166860
41	6	0	-2.491957	-4.061700	-5.768085
42	9	0	-2.844290	-1.833674	-6.417318
43	1	0	-7.601897	4.292079	-5.684219
44	1	0	-8.920004	3.358635	-4.943523
45	6	0	-6.967250	4.533247	-2.872404
46	1	0	-6.157909	0.921746	-1.653684
47	6	0	-6.092589	3.042619	-1.184801
48	6	0	-2.966932	-5.203487	-5.135840
49	9	0	-4.678767	-6.329241	-3.979230
50	9	0	-1.263326	-4.041310	-6.271836
51	1	0	-7.264240	5.526167	-3.196435
52	6	0	-6.409841	4.331335	-1.611516
53	1	0	-5.706386	2.890129	-0.181934
54	9	0	-2.181823	-6.266074	-5.026503
55	1	0	-6.250088	5.176102	-0.948827

INT2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.445869	0.567253	-0.796839
2	6	0	-4.339813	1.585757	0.182443
3	6	0	-5.498872	1.999404	0.859156
4	6	0	-6.707950	1.394152	0.551193
5	6	0	-6.797035	0.406689	-0.445017
6	6	0	-5.675823	-0.005454	-1.160178
7	1	0	-5.445275	2.780477	1.611406
8	1	0	-7.610060	1.700312	1.070535
9	1	0	-7.760464	-0.023001	-0.699920
10	6	0	-2.956938	1.973086	0.225567
11	1	0	-2.511982	2.725129	0.859918
12	6	0	-2.299372	1.198231	-0.689136
13	1	0	-1.254696	1.179942	-0.962474
14	7	0	-3.189272	0.345276	-1.301944
15	1	0	-2.964376	-0.305113	-2.040205
16	6	0	-5.795952	-0.920519	-2.302330
17	8	0	-6.596979	-2.011038	-2.081812
18	6	0	-5.236241	-0.721039	-3.513473
19	7	0	-5.405839	-1.627152	-4.600741
20	7	0	-4.665361	0.460084	-4.082424
21	6	0	-5.207451	-0.801050	-5.741159
22	6	0	-4.519580	-2.809150	-4.787230
23	7	0	-4.810105	0.383802	-5.483675
24	6	0	-4.887928	1.739052	-3.521699
25	6	0	-5.364569	-1.397187	-7.110571
26	6	0	-4.965334	-3.445155	-6.113072

27	1	0	-3.482210	-2.450880	-4.903934
28	6	0	-4.515446	-4.000327	-3.857332
29	6	0	-3.797664	2.550856	-3.217870
30	6	0	-6.158292	2.175403	-3.148772
31	1	0	-4.969679	-0.709468	-7.857532
32	1	0	-6.432713	-1.574724	-7.299954
33	8	0	-4.646517	-2.621297	-7.210954
34	1	0	-6.058893	-3.572797	-6.047750
35	6	0	-4.304369	-4.816087	-6.116565
36	6	0	-4.361399	-5.155900	-4.641504
37	6	0	-4.481553	-4.080099	-2.469598
38	6	0	-3.956701	3.729975	-2.506250
39	9	0	-2.568512	2.166785	-3.549672
40	6	0	-6.330989	3.340561	-2.418228
41	9	0	-7.226029	1.435335	-3.438124
42	1	0	-4.811956	-5.539035	-6.757922
43	1	0	-3.264372	-4.724354	-6.454128
44	6	0	-4.239381	-6.402768	-4.042606
45	1	0	-4.546885	-3.189397	-1.856192
46	6	0	-4.366074	-5.336247	-1.872559
47	6	0	-5.226284	4.118683	-2.100774
48	9	0	-2.901272	4.476525	-2.189819
49	9	0	-7.545646	3.717117	-2.025598
50	1	0	-4.131802	-7.296898	-4.649600
51	6	0	-4.254468	-6.487846	-2.650421
52	1	0	-4.355697	-5.414178	-0.790337
53	9	0	-5.383843	5.236079	-1.400230
54	1	0	-4.166222	-7.456587	-2.169024
55	1	0	-6.847542	-2.377351	-2.945416

INT3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.176113	-2.301731	-3.361235
2	6	0	-2.260618	-3.382029	-3.463044
3	6	0	-2.438524	-4.518094	-2.659010
4	6	0	-3.503183	-4.552475	-1.775594
5	6	0	-4.417567	-3.487101	-1.704600
6	6	0	-4.280686	-2.352532	-2.491916
7	1	0	-1.752917	-5.355803	-2.738071
8	1	0	-3.659703	-5.423011	-1.147116
9	1	0	-5.284208	-3.554637	-1.056615
10	6	0	-1.309196	-3.033665	-4.478569
11	1	0	-0.473767	-3.629772	-4.813205
12	6	0	-1.661140	-1.802648	-4.946033
13	1	0	-1.198750	-1.184370	-5.701070
14	7	0	-2.791924	-1.358587	-4.291376
15	1	0	-3.146825	-0.419142	-4.386791
16	6	0	-5.387597	-1.299989	-2.481630
17	1	0	-5.035506	-0.340507	-2.084058
18	8	0	-6.510770	-1.725372	-1.788348
19	6	0	-5.821586	-1.032026	-3.914205
20	7	0	-5.854059	0.105547	-4.623223
21	7	0	-6.344751	-1.964196	-4.709075
22	6	0	-6.462312	-0.199243	-5.834004
23	6	0	-5.547423	1.516906	-4.292432
24	7	0	-6.752301	-1.462484	-5.904112
25	6	0	-6.391124	-3.355796	-4.427837
26	6	0	-6.741204	0.834265	-6.896554

27	6	0	-5.472136	2.265356	-5.634850
28	1	0	-6.420165	1.887466	-3.742098
29	6	0	-4.269678	2.015936	-3.625654
30	6	0	-7.384038	-3.891085	-3.617277
31	6	0	-5.353316	-4.156994	-4.896621
32	1	0	-7.747025	0.678319	-7.287225
33	1	0	-6.016301	0.707528	-7.711464
34	8	0	-6.668260	2.136349	-6.354930
35	1	0	-4.638631	1.831908	-6.211847
36	6	0	-5.081215	3.667657	-5.201177
37	6	0	-4.074095	3.320353	-4.126573
38	6	0	-3.396257	1.511152	-2.664294
39	6	0	-7.308804	-5.223700	-3.236054
40	9	0	-8.389405	-3.144730	-3.195907
41	6	0	-5.273874	-5.484731	-4.515793
42	9	0	-4.419298	-3.628406	-5.673665
43	1	0	-4.662192	4.266569	-6.010553
44	1	0	-5.953386	4.189677	-4.789078
45	6	0	-3.034289	4.111729	-3.665303
46	1	0	-3.470582	0.511149	-2.255379
47	6	0	-2.342050	2.310536	-2.214740
48	6	0	-6.255342	-6.011694	-3.682448
49	9	0	-8.242825	-5.747172	-2.452360
50	9	0	-4.270973	-6.247715	-4.927303
51	1	0	-2.892212	5.110257	-4.066291
52	6	0	-2.166049	3.601530	-2.700209
53	1	0	-1.655275	1.908576	-1.478114
54	9	0	-6.183506	-7.279738	-3.312631
55	1	0	-1.342816	4.208084	-2.338484
56	6	0	-7.826406	0.861793	-0.055938
57	1	0	-7.719621	1.678344	0.667687
58	1	0	-8.878573	0.582177	-0.044742
59	6	0	-7.452042	1.347531	-1.449713
60	1	0	-7.656037	0.564061	-2.187577
61	1	0	-8.031461	2.235426	-1.715792
62	1	0	-6.389776	1.618501	-1.498385
63	6	0	-5.753880	0.232476	1.007409
64	1	0	-5.505609	1.106828	0.393739
65	6	0	-4.537119	-0.695026	0.914422
66	1	0	-4.511668	-1.248187	-0.028029
67	1	0	-3.629122	-0.087881	0.972843
68	1	0	-4.493221	-1.423298	1.725114
69	6	0	-5.956267	0.731162	2.441074
70	1	0	-5.048509	1.242581	2.771998
71	1	0	-6.784544	1.439275	2.523011
72	1	0	-6.143137	-0.091607	3.135329
73	6	0	-7.803845	-1.276121	1.157726
74	1	0	-8.296199	-0.737604	1.982467
75	6	0	-8.874925	-1.926364	0.272119
76	1	0	-9.507127	-2.564986	0.893782
77	1	0	-9.529322	-1.212303	-0.230089
78	1	0	-8.405611	-2.551013	-0.494105
79	6	0	-6.951617	-2.402982	1.737643
80	1	0	-6.350714	-2.865304	0.947632
81	1	0	-6.288074	-2.080334	2.538903
82	1	0	-7.614284	-3.168338	2.148578
83	7	0	-6.997963	-0.300644	0.361155
84	1	0	-6.658951	-1.134339	-0.947996

INT4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.943359	-2.254758	-2.762148
2	6	0	-2.197810	-3.303695	-2.170388
3	6	0	-2.840077	-4.159197	-1.258776
4	6	0	-4.183296	-3.952769	-0.981150
5	6	0	-4.910339	-2.924732	-1.609037
6	6	0	-4.314761	-2.063426	-2.528300
7	1	0	-2.294149	-4.968874	-0.784435
8	1	0	-4.694366	-4.606174	-0.281080
9	1	0	-5.971827	-2.814402	-1.407496
10	6	0	-0.868425	-3.215652	-2.708463
11	1	0	-0.029858	-3.856323	-2.479435
12	6	0	-0.858245	-2.153679	-3.570859
13	1	0	-0.056944	-1.759502	-4.178301
14	7	0	-2.100686	-1.563049	-3.595697
15	1	0	-2.380142	-0.800809	-4.195803
16	6	0	-5.096623	-1.032084	-3.233769
17	1	0	-5.546922	-0.136092	-1.553687
18	8	0	-5.933675	-0.248603	-2.475447
19	6	0	-5.136914	-0.922856	-4.582206
20	7	0	-5.858628	0.009477	-5.360841
21	7	0	-4.572271	-1.772885	-5.582720
22	6	0	-6.019924	-0.569530	-6.608185
23	6	0	-6.783928	1.040202	-4.928545
24	7	0	-5.295451	-1.609907	-6.794985
25	6	0	-4.208478	-3.111496	-5.315686
26	6	0	-6.980318	-0.013479	-7.633787
27	6	0	-7.373213	1.695522	-6.184473
28	1	0	-7.597291	0.581570	-4.348359
29	6	0	-6.314231	2.290083	-4.221209
30	6	0	-5.050390	-3.996595	-4.645435
31	6	0	-2.932106	-3.551416	-5.658423
32	1	0	-7.448553	-0.844770	-8.161223
33	1	0	-6.429193	0.602495	-8.358196
34	8	0	-8.001451	0.755963	-7.018963
35	1	0	-6.533509	2.153983	-6.733681
36	6	0	-8.208386	2.831031	-5.599124
37	6	0	-7.212903	3.317371	-4.557966
38	6	0	-5.219725	2.536538	-3.409809
39	6	0	-4.604111	-5.246057	-4.242426
40	9	0	-6.285234	-3.621788	-4.320329
41	6	0	-2.477929	-4.805006	-5.279539
42	9	0	-2.096881	-2.740244	-6.302545
43	1	0	-8.479823	3.595370	-6.329300
44	1	0	-9.124529	2.433959	-5.144750
45	6	0	-7.051248	4.589573	-4.028255
46	1	0	-4.514851	1.742991	-3.184275
47	6	0	-5.051169	3.824072	-2.891535
48	6	0	-3.316315	-5.649614	-4.564921
49	9	0	-5.403946	-6.059178	-3.555642
50	9	0	-1.241101	-5.195698	-5.580561
51	1	0	-7.739323	5.388909	-4.287188
52	6	0	-5.966961	4.833931	-3.181563
53	1	0	-4.195465	4.043773	-2.259279
54	9	0	-2.881161	-6.845604	-4.180675
55	1	0	-5.822532	5.825944	-2.765673
56	6	0	-5.878094	-0.742054	0.980611

57	1	0	-5.277005	-1.645329	0.840979
58	6	0	-7.285143	-1.081454	0.480543
59	1	0	-7.316228	-1.117929	-0.611756
60	1	0	-7.580815	-2.058914	0.872344
61	1	0	-8.031567	-0.358683	0.823549
62	6	0	-5.970808	1.564885	0.055378
63	1	0	-7.032545	1.329708	0.152341
64	6	0	-5.607752	2.665742	1.055274
65	1	0	-6.326933	3.482421	0.948085
66	1	0	-5.638677	2.321016	2.091442
67	1	0	-4.613396	3.080218	0.866415
68	6	0	-3.783019	0.483020	0.399394
69	1	0	-3.660423	1.118829	1.290281
70	6	0	-3.025419	-0.816872	0.665398
71	1	0	-1.959349	-0.584919	0.739039
72	1	0	-3.322112	-1.295397	1.601616
73	1	0	-3.163636	-1.529209	-0.151729
74	6	0	-3.141786	1.197623	-0.789955
75	1	0	-3.181397	0.551342	-1.676114
76	1	0	-3.641904	2.140926	-1.022851
77	1	0	-2.092717	1.417619	-0.575478
78	7	0	-5.228146	0.282674	0.127346
79	6	0	-5.914067	-0.407621	2.474917
80	1	0	-4.928940	-0.126947	2.860351
81	1	0	-6.608835	0.414770	2.673098
82	1	0	-6.262420	-1.277290	3.040255
83	1	0	-5.852351	1.967333	-0.956586

INT5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-17.467992	-4.117377	29.733206
2	6	0	-17.585632	-5.214723	30.626025
3	6	0	-18.326293	-5.064978	31.804531
4	6	0	-18.944931	-3.849725	32.080555
5	6	0	-18.793565	-2.762669	31.217549
6	6	0	-18.030499	-2.863167	30.047936
7	1	0	-18.409903	-5.893133	32.501533
8	1	0	-19.517933	-3.729628	32.992547
9	1	0	-19.209919	-1.793661	31.472624
10	6	0	-16.836953	-6.300648	30.056106
11	1	0	-16.710867	-7.288265	30.473002
12	6	0	-16.325442	-5.850118	28.876964
13	1	0	-15.719694	-6.353120	28.138411
14	7	0	-16.695969	-4.529721	28.680081
15	1	0	-16.550234	-4.038219	27.810548
16	6	0	-17.679567	-1.611896	29.378286
17	8	0	-18.305666	-0.576868	29.405560
18	6	0	-16.293676	-1.507396	28.742949
19	7	0	-15.938666	-0.834402	27.641841
20	7	0	-15.146932	-1.819762	29.360969
21	6	0	-14.560728	-0.753621	27.651228
22	6	0	-16.619787	-0.330752	26.415922
23	7	0	-14.063805	-1.353979	28.694473
24	6	0	-14.985993	-2.587912	30.545550
25	6	0	-13.761869	0.053851	26.652030
26	6	0	-15.834209	0.940678	26.051074
27	1	0	-16.407644	-1.095962	25.659948
28	6	0	-18.062427	0.099062	26.309575

29	6	0	-14.325276	-3.810844	30.469553
30	6	0	-15.588478	-2.191398	31.733673
31	1	0	-12.986460	-0.576229	26.213291
32	1	0	-13.279792	0.859987	27.220797
33	8	0	-14.548734	0.577514	25.604128
34	1	0	-15.768028	1.569514	26.952911
35	6	0	-16.706468	1.633909	25.017569
36	6	0	-18.090781	1.231306	25.480006
37	6	0	-19.244599	-0.534328	26.680151
38	6	0	-14.292171	-4.648775	31.572815
39	9	0	-13.779333	-4.199262	29.327226
40	6	0	-15.575010	-3.033957	32.833841
41	9	0	-16.241990	-1.036928	31.790348
42	1	0	-16.545281	2.712114	24.982402
43	1	0	-16.500486	1.219252	24.023597
44	6	0	-19.303346	1.795457	25.104160
45	1	0	-19.245450	-1.460521	27.242208
46	6	0	-20.457522	0.037737	26.303270
47	6	0	-14.922162	-4.258377	32.749281
48	9	0	-13.691133	-5.826652	31.502280
49	9	0	-16.183652	-2.680948	33.955680
50	1	0	-19.323201	2.678970	24.473980
51	6	0	-20.487471	1.203154	25.537121
52	1	0	-21.386002	-0.435193	26.604141
53	9	0	-14.916372	-5.068019	33.793914
54	1	0	-21.441263	1.637721	25.256631

INT6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-17.149948	-2.713893	27.592650
2	6	0	-15.949130	-3.516153	27.566887
3	6	0	-14.853159	-3.075744	26.828493
4	6	0	-14.920376	-1.870819	26.110847
5	6	0	-16.084033	-1.106769	26.099015
6	6	0	-17.216473	-1.528918	26.816131
7	1	0	-13.942170	-3.668453	26.790172
8	1	0	-14.062686	-1.547240	25.530773
9	1	0	-16.156295	-0.210974	25.489601
10	6	0	-16.265907	-4.652175	28.371747
11	1	0	-15.625032	-5.487431	28.617223
12	6	0	-17.564100	-4.437742	28.798818
13	1	0	-18.150499	-5.094794	29.433082
14	7	0	-18.119618	-3.264420	28.345376
15	6	0	-18.487143	-0.891423	26.589192
16	8	0	-18.728745	0.210786	26.127895
17	6	0	-19.723252	-1.773522	26.789917
18	7	0	-20.853039	-1.497248	27.443358
19	7	0	-19.993529	-2.842366	26.031480
20	6	0	-21.775260	-2.461938	27.070984
21	6	0	-21.189678	-0.661176	28.618666
22	7	0	-21.266005	-3.291659	26.213683
23	6	0	-19.023812	-3.639064	25.371365
24	6	0	-23.214276	-2.442229	27.532042
25	6	0	-22.695758	-0.393640	28.486837
26	1	0	-21.018443	-1.318592	29.480761
27	6	0	-20.629522	0.710585	28.915960
28	6	0	-18.760915	-4.915981	25.863523
29	6	0	-18.200868	-3.091212	24.395480

30	1	0	-23.517228	-3.451456	27.813091
31	1	0	-23.825023	-2.112821	26.680242
32	8	0	-23.413655	-1.595018	28.644714
33	1	0	-22.874142	0.027086	27.484168
34	6	0	-22.969845	0.678575	29.528220
35	6	0	-21.677426	1.465794	29.469151
36	6	0	-19.328959	1.203558	28.917311
37	6	0	-17.666615	-5.626054	25.398250
38	9	0	-19.534851	-5.449389	26.795105
39	6	0	-17.095188	-3.791068	23.938994
40	9	0	-18.428570	-1.860317	23.947592
41	1	0	-23.860677	1.268733	29.308085
42	1	0	-23.094132	0.213541	30.513713
43	6	0	-21.444866	2.748945	29.945783
44	1	0	-18.490978	0.608589	28.577345
45	6	0	-19.103401	2.495415	29.390950
46	6	0	-16.832035	-5.057369	24.443497
47	9	0	-17.405305	-6.839566	25.867666
48	9	0	-16.291969	-3.252894	23.029026
49	1	0	-22.258297	3.333867	30.363999
50	6	0	-20.152407	3.267387	29.887773
51	1	0	-18.095754	2.896730	29.379614
52	9	0	-15.776408	-5.730614	24.010012
53	1	0	-19.957640	4.271517	30.250135

***Re*-INT7**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-18.796779	-1.374764	26.143252
2	6	0	-17.977209	-1.994049	27.104932
3	6	0	-16.587516	-1.812547	26.978805
4	6	0	-16.110657	-1.011452	25.950625
5	6	0	-16.973381	-0.394335	25.017598
6	6	0	-18.340877	-0.593191	25.085647
7	1	0	-15.898479	-2.282009	27.673791
8	1	0	-15.041037	-0.858108	25.850994
9	1	0	-16.557030	0.215026	24.219607
10	6	0	-18.874630	-2.684501	27.994925
11	1	0	-18.609698	-3.289902	28.849147
12	6	0	-20.151506	-2.435642	27.562236
13	1	0	-21.097136	-2.762041	27.969069
14	7	0	-20.106246	-1.657225	26.420053
15	6	0	-19.355282	0.008028	24.103142
16	8	0	-19.411465	1.272252	24.058266
17	6	0	-19.086421	-0.629084	22.674340
18	7	0	-19.019878	0.038417	21.508635
19	7	0	-18.641006	-1.856990	22.385523
20	6	0	-18.476373	-0.817747	20.580942
21	6	0	-19.406506	1.445384	21.202657
22	7	0	-18.240252	-1.989414	21.090852
23	6	0	-18.540623	-2.940884	23.290946
24	6	0	-18.119572	-0.347784	19.206867
25	6	0	-18.998801	1.782927	19.730747
26	1	0	-18.889742	2.050506	21.945315
27	6	0	-20.903494	1.674114	21.193262
28	6	0	-19.692910	-3.590310	23.715986
29	6	0	-17.299441	-3.296256	23.809596
30	1	0	-18.896780	-0.629841	18.487523
31	1	0	-17.186588	-0.824384	18.903771

32	8	0	-17.895104	1.042519	19.248467
33	1	0	-18.657911	2.819760	19.741161
34	6	0	-20.278438	1.684581	18.874277
35	6	0	-21.380010	1.822190	19.889132
36	6	0	-21.756216	1.798151	22.287216
37	6	0	-19.615819	-4.538294	24.727173
38	9	0	-20.854196	-3.308984	23.149393
39	6	0	-17.217274	-4.241563	24.816778
40	9	0	-16.203040	-2.699446	23.364523
41	1	0	-20.301388	2.464330	18.109540
42	1	0	-20.350497	0.726086	18.350425
43	6	0	-22.728832	2.077501	19.658574
44	1	0	-21.344457	1.705998	23.286060
45	6	0	-23.105642	2.050175	22.051081
46	6	0	-18.380774	-4.843051	25.285157
47	9	0	-20.704171	-5.165708	25.155283
48	9	0	-16.046150	-4.556378	25.357570
49	1	0	-23.101326	2.197953	18.645769
50	6	0	-23.590133	2.184193	20.747782
51	1	0	-23.788588	2.158921	22.888830
52	9	0	-18.305202	-5.736486	26.260638
53	1	0	-24.643951	2.384934	20.581913
54	6	0	-21.105674	-0.870299	25.703917
55	8	0	-20.697263	-0.740572	24.378650
56	6	0	-22.403886	-1.705231	25.669752
57	9	0	-23.277497	-1.219355	24.788089
58	9	0	-22.164187	-2.979597	25.349570
59	9	0	-22.990188	-1.706637	26.878055
60	6	0	-21.370074	0.474748	26.387126
61	6	0	-20.735433	0.827299	27.574808
62	6	0	-22.271306	1.364017	25.796157
63	6	0	-20.993961	2.064362	28.164228
64	1	0	-20.033075	0.144638	28.043605
65	6	0	-22.531116	2.594355	26.386876
66	1	0	-22.764538	1.086291	24.871024
67	6	0	-21.889825	2.949065	27.573738
68	1	0	-20.489037	2.333642	29.086158
69	1	0	-23.231719	3.278688	25.918741
70	1	0	-22.088010	3.911703	28.033859

***Si*-INT7**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-18.983238	-1.508504	25.723074
2	6	0	-18.357764	-2.635314	26.286751
3	6	0	-16.976381	-2.791521	26.069944
4	6	0	-16.301857	-1.828062	25.332938
5	6	0	-16.967988	-0.713574	24.779391
6	6	0	-18.331871	-0.553843	24.948496
7	1	0	-16.446359	-3.651610	26.467637
8	1	0	-15.235442	-1.937703	25.164697
9	1	0	-16.416733	0.013169	24.189611
10	6	0	-19.401936	-3.369923	26.952509
11	1	0	-19.307282	-4.310054	27.475940
12	6	0	-20.564151	-2.665892	26.789383
13	1	0	-21.559904	-2.902986	27.129478
14	7	0	-20.325086	-1.534660	26.025802
15	6	0	-19.127069	0.577069	24.304590
16	8	0	-18.721598	1.760569	24.489592

17	6	0	-19.294284	0.281024	22.763283
18	7	0	-19.410867	1.220646	21.810098
19	7	0	-19.153337	-0.868658	22.096089
20	6	0	-19.267508	0.588317	20.597004
21	6	0	-19.692032	2.681151	21.957971
22	7	0	-19.121467	-0.694779	20.741816
23	6	0	-19.155530	-2.177251	22.641753
24	6	0	-19.218176	1.351343	19.307899
25	6	0	-19.874379	3.265922	20.530277
26	1	0	-18.850634	3.097402	22.507746
27	6	0	-21.044106	2.959770	22.584202
28	6	0	-20.337423	-2.703528	23.152144
29	6	0	-17.982546	-2.920723	22.702169
30	1	0	-20.134240	1.181112	18.730512
31	1	0	-18.373462	0.990204	18.718889
32	8	0	-18.994944	2.715763	19.571243
33	1	0	-19.606311	4.322726	20.593977
34	6	0	-21.380917	3.152460	20.216474
35	6	0	-21.993918	3.217141	21.590055
36	6	0	-21.384847	3.025536	23.932599
37	6	0	-20.343343	-3.952342	23.753124
38	9	0	-21.458799	-1.999191	23.094219
39	6	0	-17.983814	-4.172113	23.296141
40	9	0	-16.852601	-2.413763	22.231316
41	1	0	-21.715203	3.952117	19.551913
42	1	0	-21.631363	2.202064	19.731712
43	6	0	-23.311497	3.504108	21.930592
44	1	0	-20.633679	2.831965	24.687014
45	6	0	-22.707572	3.306644	24.269305
46	6	0	-19.164036	-4.681101	23.825249
47	9	0	-21.461126	-4.438939	24.279670
48	9	0	-16.855826	-4.864282	23.405364
49	1	0	-24.049263	3.705532	21.159670
50	6	0	-23.663975	3.536529	23.278859
51	1	0	-22.994068	3.340607	25.315232
52	9	0	-19.156137	-5.859985	24.429771
53	1	0	-24.689754	3.754026	23.560583
54	6	0	-23.366753	-1.065062	26.712421
55	6	0	-22.598954	-0.536016	25.669430
56	6	0	-23.232562	-0.157032	24.484450
57	6	0	-24.605198	-0.330689	24.334516
58	6	0	-25.361974	-0.882968	25.364070
59	6	0	-24.738454	-1.246225	26.554127
60	1	0	-22.913481	-1.317987	27.663225
61	1	0	-22.642757	0.283744	23.689879
62	1	0	-25.083208	-0.025280	23.408967
63	1	0	-26.431972	-1.019776	25.244542
64	1	0	-25.318484	-1.663313	27.370824
65	6	0	-21.089879	-0.301433	25.802933
66	8	0	-20.635693	0.306690	24.648879
67	6	0	-20.828639	0.640188	27.007979
68	9	0	-19.543106	0.980549	27.114663
69	9	0	-21.540723	1.766827	26.887279
70	9	0	-21.172831	0.059239	28.170788

***R*-P**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-19.347357	-1.357869	25.748269

2	6	0	-18.566494	-2.293056	26.442050
3	6	0	-17.175862	-2.190471	26.276555
4	6	0	-16.655952	-1.189565	25.457130
5	6	0	-17.478322	-0.278262	24.771796
6	6	0	-18.856651	-0.362318	24.915707
7	1	0	-16.505336	-2.879609	26.780164
8	1	0	-15.580950	-1.115193	25.336040
9	1	0	-17.050776	0.479466	24.124101
10	6	0	-19.506527	-3.124188	27.156835
11	1	0	-19.278987	-3.964889	27.794705
12	6	0	-20.761376	-2.664736	26.870894
13	1	0	-21.729121	-3.010692	27.204342
14	7	0	-20.666770	-1.589424	25.994635
15	6	0	-19.856833	0.446904	24.207770
16	8	0	-19.642306	1.319969	23.413373
17	6	0	-24.129444	-1.234325	25.896682
18	6	0	-22.947775	-1.327289	25.163499
19	6	0	-22.895491	-2.128618	24.019802
20	6	0	-24.022732	-2.824453	23.604480
21	6	0	-25.207705	-2.729175	24.334246
22	6	0	-25.257457	-1.938047	25.476375
23	1	0	-24.190775	-0.622547	26.788428
24	1	0	-21.968337	-2.195660	23.458531
25	1	0	-23.978742	-3.440606	22.712885
26	1	0	-26.089455	-3.273001	24.011704
27	1	0	-26.176415	-1.862161	26.047535
28	6	0	-21.658204	-0.629787	25.556359
29	8	0	-21.182491	0.084519	24.419676
30	6	0	-21.834133	0.429662	26.665094
31	9	0	-20.683950	1.087886	26.851785
32	9	0	-22.771232	1.320289	26.346517
33	9	0	-22.169147	-0.145397	27.825489

***S*-P**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-19.545198	-1.599880	25.824093
2	6	0	-18.798428	-2.295190	26.785276
3	6	0	-17.409001	-2.098233	26.762818
4	6	0	-16.855758	-1.236986	25.815711
5	6	0	-17.640584	-0.566499	24.862531
6	6	0	-19.018287	-0.747297	24.861148
7	1	0	-16.765162	-2.604726	27.474789
8	1	0	-15.781959	-1.087072	25.805901
9	1	0	-17.183117	0.078340	24.119839
10	6	0	-19.766536	-3.037617	27.557148
11	1	0	-19.569091	-3.711080	28.377550
12	6	0	-21.004231	-2.750295	27.053739
13	1	0	-21.977504	-3.100085	27.362166
14	7	0	-20.871147	-1.882945	25.969811
15	6	0	-19.957908	-0.232563	23.854343
16	8	0	-19.690402	0.425537	22.887119
17	6	0	-21.781777	-0.974353	25.300267
18	8	0	-21.267167	-0.664192	24.011543
19	6	0	-23.097407	-1.712927	25.002145
20	9	0	-23.918580	-0.952657	24.282400
21	9	0	-22.874403	-2.843229	24.336136
22	9	0	-23.709975	-2.019786	26.153732
23	6	0	-22.037595	0.308746	26.083810

24	6	0	-21.802370	0.379759	27.455968
25	6	0	-22.528041	1.423612	25.399066
26	6	0	-22.060171	1.564144	28.141639
27	1	0	-21.406097	-0.477318	27.991595
28	6	0	-22.783571	2.603294	26.089403
29	1	0	-22.695749	1.366431	24.328847
30	6	0	-22.552275	2.674522	27.461739
31	1	0	-21.869738	1.617587	29.208195
32	1	0	-23.159104	3.468614	25.553600
33	1	0	-22.750270	3.596481	27.998455

***Si*-TS1′**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.806642	-2.397507	-0.384062
2	6	0	-1.436160	-2.213617	-0.183386
3	6	0	-0.860321	-0.981187	-0.502775
4	6	0	-1.631059	0.046059	-1.032191
5	6	0	-2.998432	-0.141261	-1.232251
6	6	0	-3.582200	-1.359900	-0.902151
7	1	0	-3.285773	-3.338812	-0.139356
8	1	0	0.198901	-0.838231	-0.309363
9	1	0	-1.168890	0.996297	-1.279946
10	1	0	-3.605248	0.660648	-1.640179
11	1	0	-4.647095	-1.512166	-1.049484
12	6	0	-0.490266	-3.255884	0.434430
13	8	0	0.417403	-2.831583	1.192740
14	6	0	-1.218802	-4.515930	0.951105
15	9	0	-0.370558	-5.429761	1.430352
16	9	0	-2.039957	-4.166527	1.952073
17	9	0	-1.973995	-5.145803	0.028632
18	6	0	0.312832	-3.829216	-1.161792
19	7	0	1.563825	-3.369794	-1.413869
20	7	0	-0.219564	-3.929297	-2.393130
21	6	0	1.675214	-3.133656	-2.773808
22	6	0	2.669571	-2.944861	-0.529390
23	7	0	0.596678	-3.484657	-3.398497
24	6	0	-1.531156	-4.326082	-2.741180
25	6	0	2.877871	-2.498447	-3.426379
26	6	0	3.912618	-2.785820	-1.419999
27	1	0	2.376134	-1.975581	-0.110656
28	6	0	3.261278	-3.802521	0.569733
29	6	0	-2.407793	-3.385863	-3.272428
30	6	0	-1.947125	-5.641872	-2.584558
31	1	0	2.531986	-1.742824	-4.132819
32	1	0	3.441073	-3.266452	-3.973672
33	8	0	3.698103	-1.869679	-2.463614
34	1	0	4.133781	-3.777282	-1.849998
35	6	0	5.008630	-2.467478	-0.414806
36	6	0	4.620921	-3.457863	0.664932
37	6	0	2.704737	-4.734253	1.430478
38	6	0	-3.704722	-3.745258	-3.604530
39	9	0	-2.016984	-2.130712	-3.426817
40	6	0	-3.242532	-6.009951	-2.915084
41	9	0	-1.119574	-6.545478	-2.080370
42	1	0	6.013770	-2.619319	-0.811146
43	1	0	4.916676	-1.430038	-0.070235
44	6	0	5.429166	-4.040126	1.630706
45	1	0	1.654123	-4.973861	1.372127

46	6	0	3.526194	-5.329531	2.389907
47	6	0	-4.117265	-5.059834	-3.428018
48	9	0	-4.552436	-2.835430	-4.072431
49	9	0	-3.646332	-7.265066	-2.751645
50	1	0	6.480380	-3.776831	1.700308
51	6	0	4.871803	-4.982568	2.495927
52	1	0	3.106616	-6.066668	3.066927
53	9	0	-5.356363	-5.409903	-3.741924
54	1	0	5.492353	-5.453021	3.252017

***Re*-TS1′**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.351961	-2.950384	-0.859546
2	6	0	-1.266111	-3.735757	-1.256644
3	6	0	-1.257031	-4.281646	-2.541003
4	6	0	-2.288497	-4.016697	-3.434147
5	6	0	-3.365141	-3.222978	-3.038654
6	6	0	-3.396859	-2.699834	-1.749100
7	1	0	-2.399930	-2.525397	0.136643
8	1	0	-0.416481	-4.899974	-2.841384
9	1	0	-2.255205	-4.429301	-4.437361
10	1	0	-4.172426	-3.013328	-3.733036
11	1	0	-4.235295	-2.087886	-1.430792
12	6	0	-0.091408	-4.101658	-0.351148
13	8	0	0.282486	-5.297074	-0.299796
14	6	0	-0.159325	-3.442682	1.058532
15	9	0	-1.193672	-3.957055	1.734365
16	9	0	-0.316350	-2.102747	1.055998
17	9	0	0.951378	-3.698601	1.761846
18	6	0	1.310005	-2.974721	-0.962965
19	7	0	2.589762	-3.178558	-0.587089
20	7	0	1.274016	-1.653275	-1.189300
21	6	0	3.227027	-1.953795	-0.509664
22	6	0	3.291298	-4.400709	-0.170326
23	7	0	2.440585	-0.997546	-0.900658
24	6	0	0.169777	-0.941119	-1.711263
25	6	0	4.628132	-1.785725	0.028671
26	6	0	4.787383	-4.054484	-0.143406
27	1	0	2.934400	-4.644952	0.836640
28	6	0	3.351844	-5.648510	-1.025802
29	6	0	-0.472460	0.037468	-0.960961
30	6	0	-0.293702	-1.243748	-2.988266
31	1	0	4.632681	-0.964074	0.746093
32	1	0	5.309019	-1.541093	-0.797595
33	8	0	5.054404	-2.959339	0.695840
34	1	0	5.073109	-3.790970	-1.175580
35	6	0	5.431408	-5.399159	0.168521
36	6	0	4.589556	-6.260226	-0.757825
37	6	0	2.458231	-6.206240	-1.925124
38	6	0	-1.596444	0.675570	-1.465598
39	9	0	-0.025578	0.359774	0.244016
40	6	0	-1.423478	-0.620032	-3.491918
41	9	0	0.336670	-2.147305	-3.727361
42	1	0	6.498463	-5.430465	-0.056627
43	1	0	5.282208	-5.659736	1.223376
44	6	0	4.925671	-7.456635	-1.374973
45	1	0	1.497100	-5.739682	-2.098668
46	6	0	2.809001	-7.402134	-2.554289

47	6	0	-2.073659	0.338327	-2.725573
48	9	0	-2.222959	1.598643	-0.744366
49	9	0	-1.887676	-0.934871	-4.694961
50	1	0	5.882534	-7.930148	-1.176860
51	6	0	4.023630	-8.026273	-2.275926
52	1	0	2.123245	-7.851869	-3.264995
53	9	0	-3.159471	0.932518	-3.199726
54	1	0	4.276241	-8.957369	-2.773147

***Si*-INT1′**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.935748	-2.584992	-0.472867
2	6	0	-1.603611	-2.300653	-0.166114
3	6	0	-1.155840	-0.980000	-0.256985
4	6	0	-2.004346	0.033113	-0.685676
5	6	0	-3.328105	-0.259690	-1.012728
6	6	0	-3.791303	-1.565728	-0.894885
7	1	0	-3.324885	-3.594164	-0.399456
8	1	0	-0.131501	-0.766615	0.033650
9	1	0	-1.636587	1.051638	-0.760806
10	1	0	-3.995818	0.527566	-1.347829
11	1	0	-4.824834	-1.800552	-1.131140
12	6	0	-0.531585	-3.319262	0.329365
13	8	0	0.223368	-2.857169	1.285336
14	6	0	-1.184699	-4.670381	0.715555
15	9	0	-0.259777	-5.569852	1.082308
16	9	0	-2.022850	-4.504700	1.739957
17	9	0	-1.887079	-5.265425	-0.279322
18	6	0	0.376888	-3.591150	-0.968686
19	7	0	1.694534	-3.290481	-1.019789
20	7	0	0.022263	-3.777351	-2.248982
21	6	0	2.036085	-3.217859	-2.361357
22	6	0	2.686527	-2.827574	-0.000787
23	7	0	1.037117	-3.529538	-3.124575
24	6	0	-1.247270	-4.086965	-2.803835
25	6	0	3.363577	-2.725309	-2.877285
26	6	0	4.049269	-2.769153	-0.720077
27	1	0	2.357168	-1.823569	0.283208
28	6	0	3.116448	-3.582952	1.251677
29	6	0	-2.034537	-3.063700	-3.318303
30	6	0	-1.661768	-5.407352	-2.929804
31	1	0	3.177618	-2.079645	-3.736222
32	1	0	3.977474	-3.578498	-3.195583
33	8	0	4.020151	-1.977412	-1.879350
34	1	0	4.311928	-3.803294	-0.998790
35	6	0	4.996695	-2.343300	0.385902
36	6	0	4.456210	-3.224250	1.490591
37	6	0	2.454848	-4.425521	2.133181
38	6	0	-3.265991	-3.348086	-3.887400
39	9	0	-1.631848	-1.807958	-3.223001
40	6	0	-2.887064	-5.701208	-3.506824
41	9	0	-0.901332	-6.388222	-2.469465
42	1	0	6.045022	-2.529707	0.147551
43	1	0	4.866483	-1.276792	0.607349
44	6	0	5.135354	-3.701393	2.602694
45	1	0	1.413610	-4.654562	1.979734
46	6	0	3.148590	-4.917904	3.240026
47	6	0	-3.684087	-4.668719	-3.987565

48	9	0	-4.041984	-2.366149	-4.330503
49	9	0	-3.293764	-6.960411	-3.618396
50	1	0	6.170291	-3.420789	2.774484
51	6	0	4.472974	-4.558376	3.480175
52	1	0	2.639656	-5.584253	3.929365
53	9	0	-4.855084	-4.948159	-4.538953
54	1	0	4.991344	-4.948085	4.350618

***Re*-INT1′**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.365838	-3.053053	-1.044986
2	6	0	-1.186439	-3.718813	-1.392403
3	6	0	-1.015853	-4.138011	-2.712916
4	6	0	-1.967753	-3.848836	-3.684520
5	6	0	-3.132121	-3.165539	-3.336854
6	6	0	-3.331741	-2.781247	-2.013566
7	1	0	-2.544398	-2.726261	-0.027147
8	1	0	-0.108700	-4.673837	-2.976617
9	1	0	-1.804166	-4.159444	-4.711637
10	1	0	-3.879125	-2.939455	-4.091018
11	1	0	-4.240517	-2.259402	-1.729433
12	6	0	-0.040147	-4.094531	-0.421123
13	8	0	0.348333	-5.335246	-0.470026
14	6	0	-0.415715	-3.728231	1.051681
15	9	0	-1.472507	-4.436006	1.452028
16	9	0	-0.706224	-2.420907	1.253303
17	9	0	0.603813	-4.012036	1.878486
18	6	0	1.186604	-3.084757	-0.653289
19	7	0	2.462258	-3.373937	-0.329744
20	7	0	1.174862	-1.755736	-0.822434
21	6	0	3.128986	-2.168063	-0.196251
22	6	0	3.141040	-4.641751	0.039433
23	7	0	2.368348	-1.168688	-0.525144
24	6	0	0.111832	-0.963402	-1.325356
25	6	0	4.512420	-2.042354	0.394181
26	6	0	4.633466	-4.296826	0.198042
27	1	0	2.703833	-4.948999	0.994451
28	6	0	3.290829	-5.846695	-0.878934
29	6	0	-0.587400	-0.092466	-0.498681
30	6	0	-0.216705	-1.052089	-2.674940
31	1	0	4.505270	-1.216377	1.106356
32	1	0	5.241008	-1.827287	-0.398399
33	8	0	4.852289	-3.228199	1.082402
34	1	0	5.000720	-4.007126	-0.800515
35	6	0	5.250110	-5.649312	0.516225
36	6	0	4.503944	-6.464558	-0.522698
37	6	0	2.497812	-6.377956	-1.884622
38	6	0	-1.663735	0.623909	-1.002589
39	9	0	-0.239779	0.058386	0.769486
40	6	0	-1.299988	-0.352650	-3.179599
41	9	0	0.493717	-1.831933	-3.477543
42	1	0	6.333727	-5.668939	0.391318
43	1	0	5.002859	-5.953421	1.540512
44	6	0	4.916138	-7.629347	-1.154621
45	1	0	1.542873	-5.921441	-2.106182
46	6	0	2.927691	-7.539234	-2.529184
47	6	0	-2.021972	0.484307	-2.337525
48	9	0	-2.345114	1.448664	-0.216373

49	9	0	-1.643629	-0.472548	-4.455265
50	1	0	5.854455	-8.101216	-0.878706
51	6	0	4.117489	-8.166216	-2.164552
52	1	0	2.317805	-7.963927	-3.320243
53	9	0	-3.056703	1.159692	-2.813503
54	1	0	4.429337	-9.072141	-2.674727