Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Influence of hydrogen bonds on the reaction of guanine and hydroxyl radical: DFT calculation in C(H$^+$)GC motif

Yinghui Wang* Simin Wei*

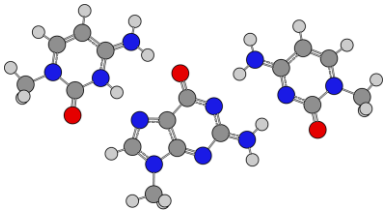

Figure S1 Optimized geometries of Tri-G(N1-H)• obtained at IEFPCM/M06-2X/6-31++G(d,p) level of theory. Oxygen, nitrogen carbon and hydrogen atoms are denoted with red, blue, gray and white balls, respectively.

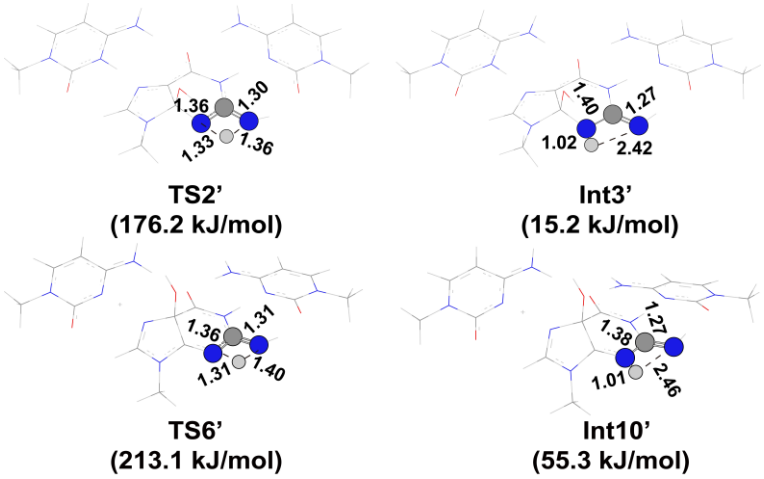

Figure S2 Optimized geometries of the related species for the direct HT of adduct radicals (Int2 and Int9) obtained at IEFPCM/M06-2X/6-31++G(d,p) level of theory. Oxygen, nitrogen carbon and hydrogen atoms are denoted with red, blue, gray and white balls, respectively.

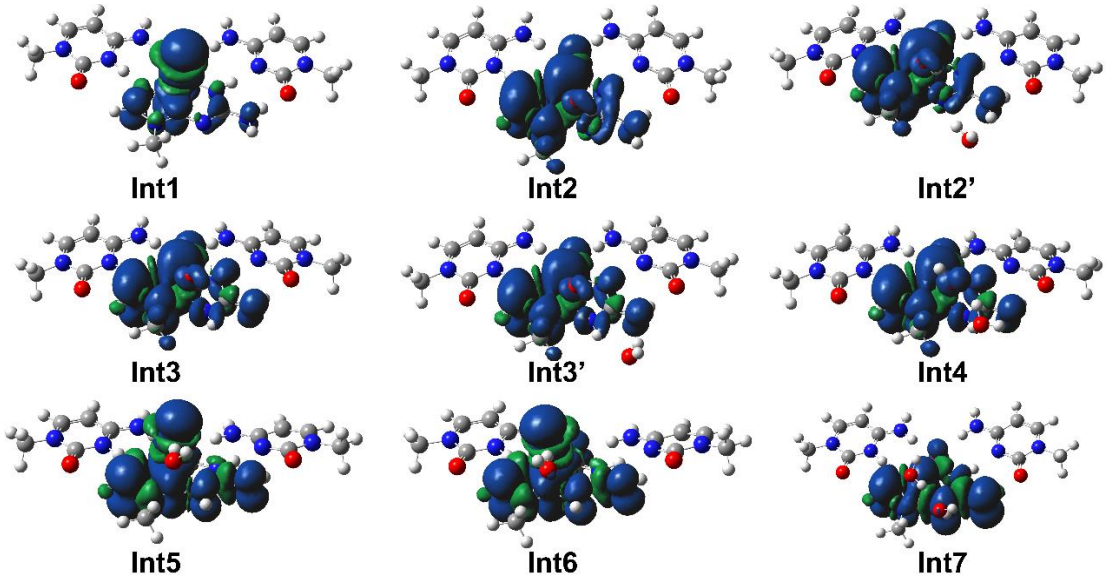

Figure S3 Spin density distribution for optimized structures of related intermediates in C4 addition/elimination pathway at the IEFPCM/M06-2X/6-31++G(d,p) level of theory.

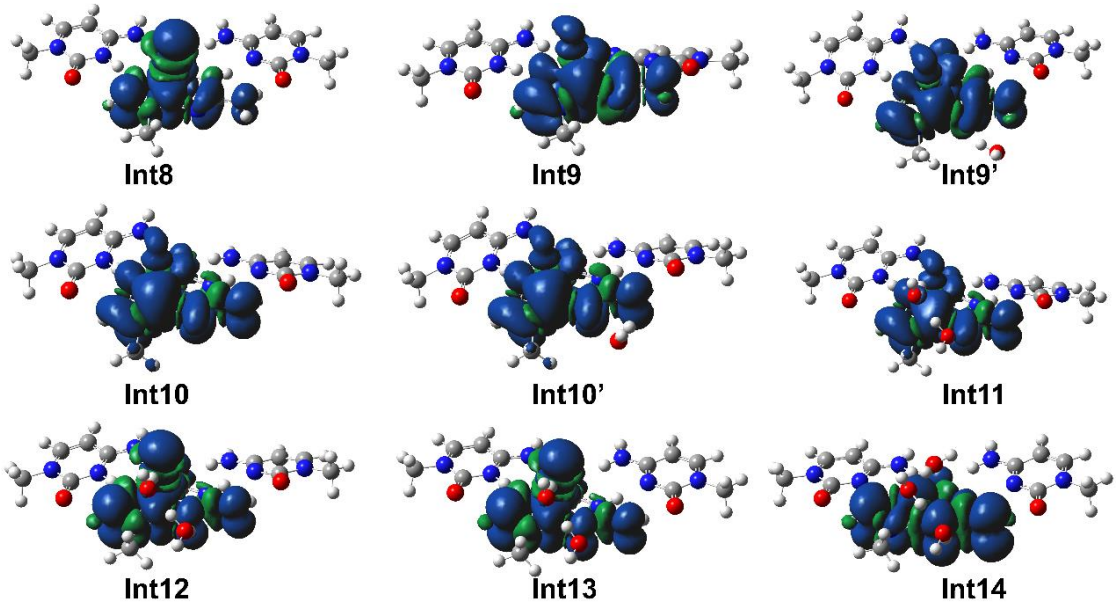

Figure S4 Spin density distribution for optimized structures of related intermediates in C5 addition/elimination pathway at the IEFPCM/M06-2X/6-31++G(d,p) level of theory.

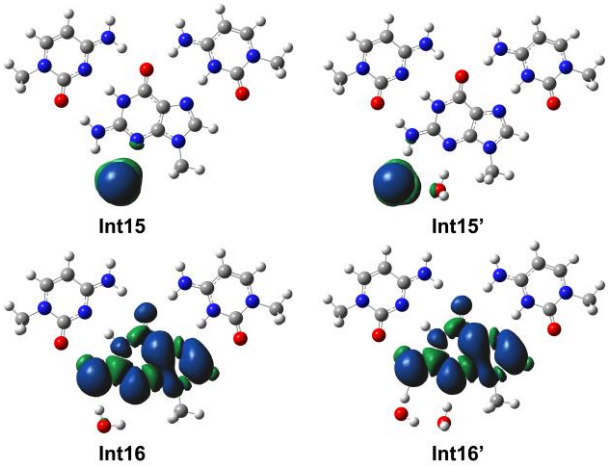

Figure S5 Spin density distribution for optimized structures of related intermediates in N2-H abstraction pathway at the IEFPCM/M06-2X/6-31++G(d,p) level of theory.

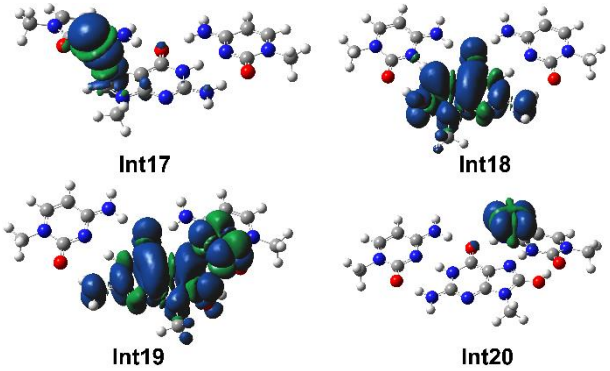

Figure S6 Spin density distribution for optimized structures of related intermediates in C8 addition pathway at the IEFPCM/M06-2X/6-31++G(d,p) level of theory.

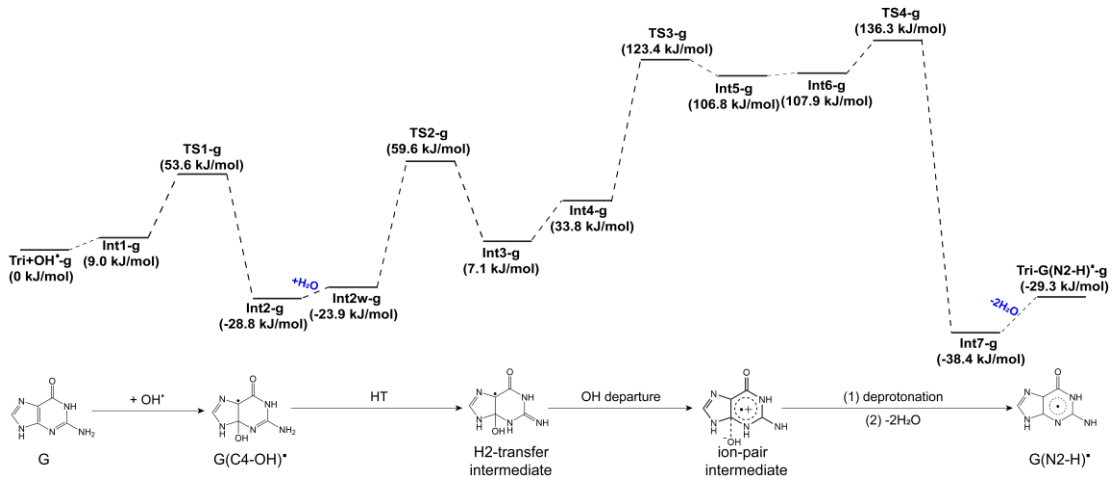

Figure S7 Relative energies obtained at M06-2X/6-311++G(d,p) level of theory in gas phase for related species along with C4 pathway down to G(N2–H)• in Tri.

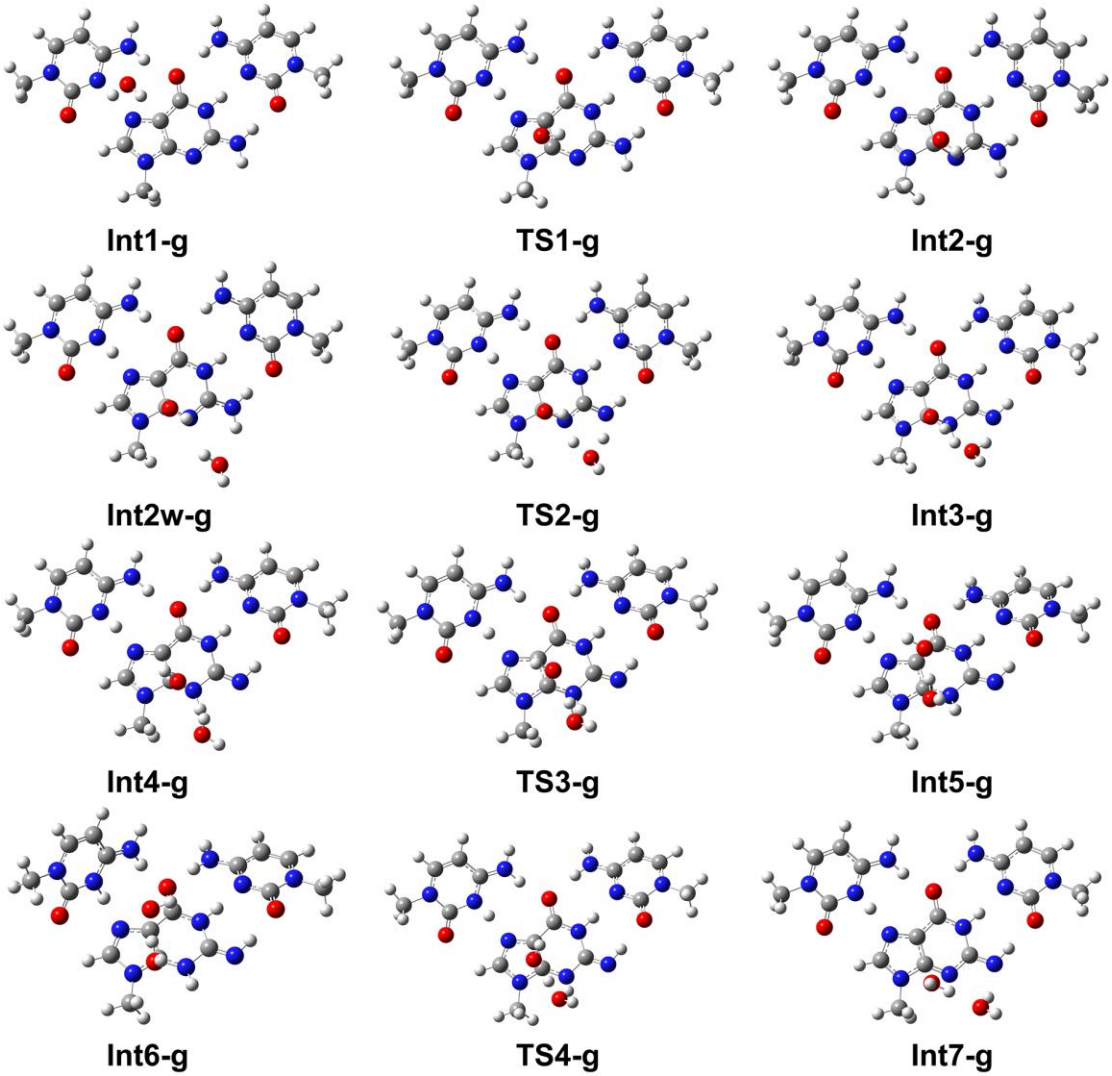

Figure S8 Optimized geometries obtained at M06-2X/6-31++G(d,p) level of theory in gas phase for related species along with C4 pathway down to G(N2–H)• in Tri. Oxygen, nitrogen, carbon and hydrogen atoms are denoted with red, blue, gray and white balls, respectively.

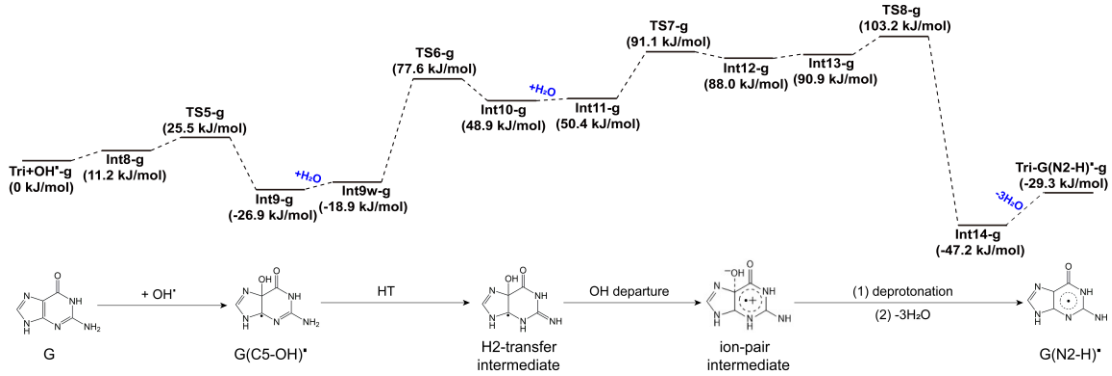

Figure S9 Relative energies obtained at M06-2X/6-311++G(d,p) level of theory in gas phase for related species along with C5 pathway down to G(N2–H)• in Tri.

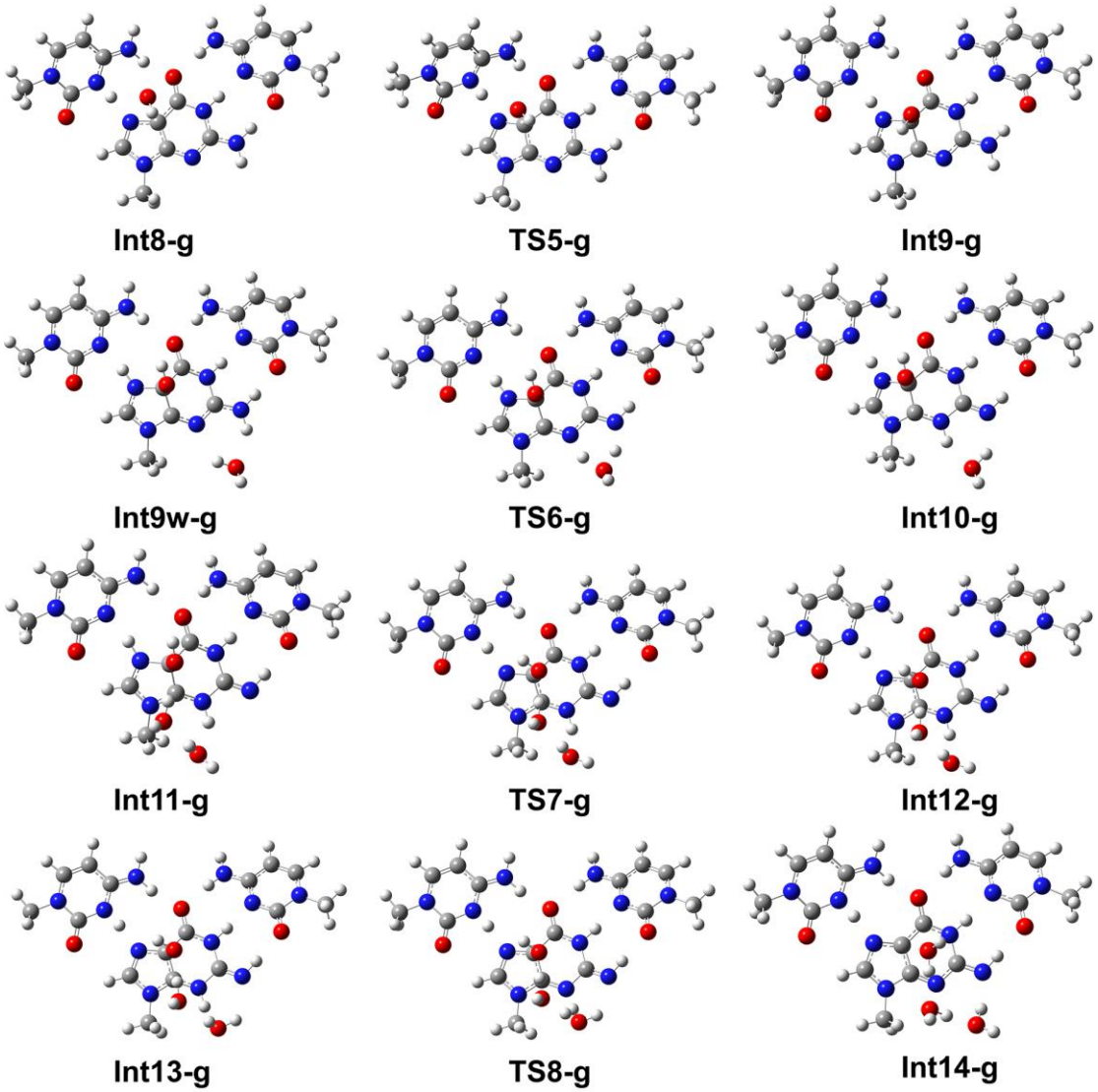

Figure S10 Optimized geometries obtained at M06-2X/6-31++G(d,p) level of theory in gas phase for related species along with C5 pathway down to G(N2–H)• in Tri. Oxygen, nitrogen, carbon and hydrogen atoms are denoted with red, blue, gray and white balls, respectively.

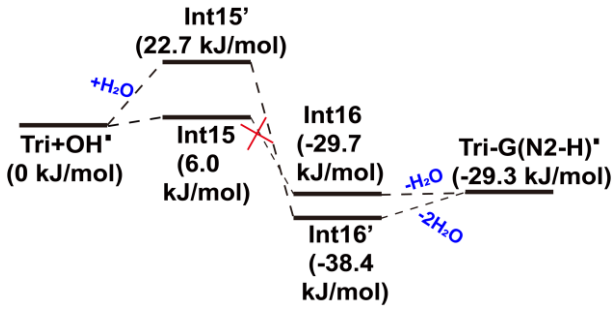

Figure S11 Relative energies obtained at M06-2X/6-311++G(d,p) level of theory in gas phase for related species along with hydrogen abstraction from N2 in Tri.

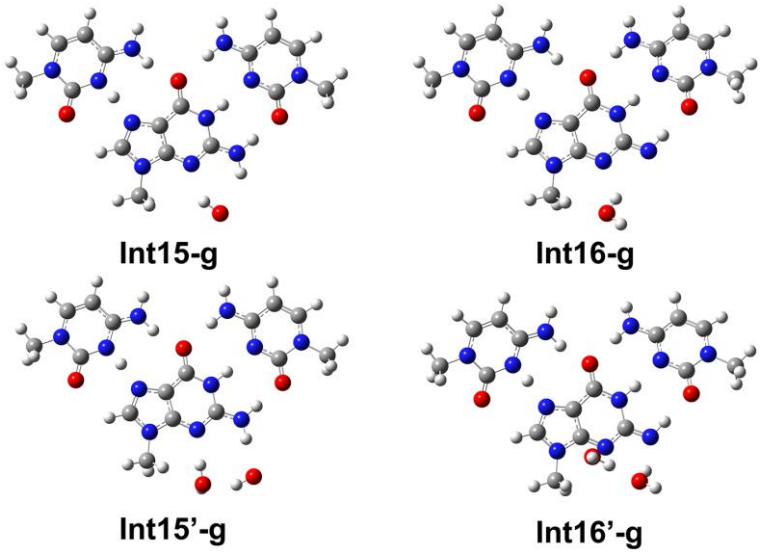

Figure S12 Optimized geometries obtained at M06-2X/6-31++G(d,p) level of theory in gas phase for related species along with hydrogen abstraction from N2 in Tri. Oxygen, nitrogen, carbon and hydrogen atoms are denoted with red, blue, gray and white balls, respectively.

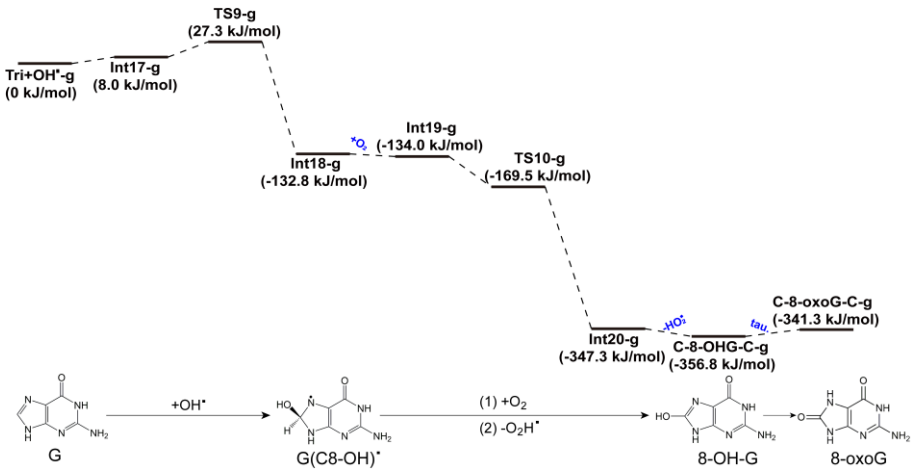

Figure S13 Relative energies obtained at M06-2X/6-311++G(d,p) level of theory in gas phase for related species along with C8 pathway down to 8-oxoG in Tri.

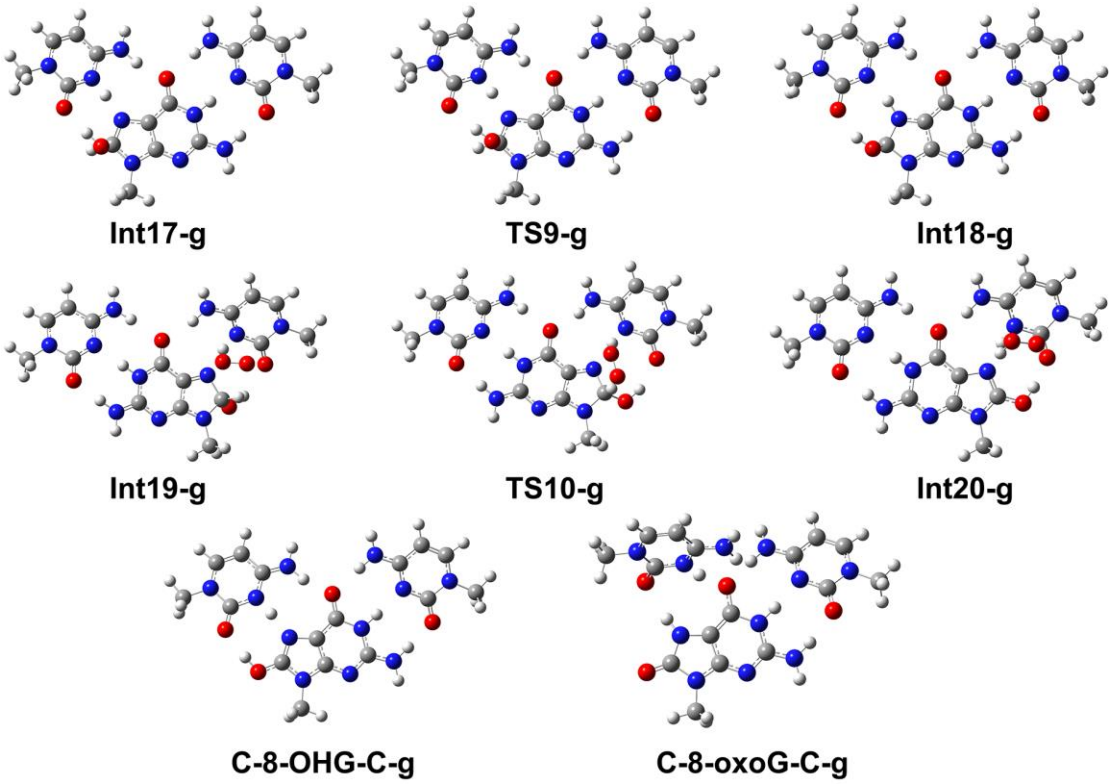

Figure S14 Optimized geometries obtained at M06-2X/6-31++G(d,p) level of theory in gas phase for related species along with C8 pathway down to 8-oxoG in Tri. Oxygen, nitrogen, carbon and hydrogen atoms are denoted with red, blue, gray and white balls, respectively.

Table S1 Mulliken charge distribution (|e|) of related species obtained at IEFPCM/M06-2X/6-31++G(d,p) level of theory.

	HO•	G	GC	C(H^+)GC	Int1	Int8	Int17
C4	-	-0.157	-0.123	-0.208	-0.175	-0.134	-0.167
C5	-	-0.236	-0.063	-0.347	-0.685	-1.034	-0.226
C8	-	0.392	0.490	0.352	0.451	0.492	0.230
O (HO•)	-0.378	-	-	-	-0.345	-0.479	-0.378

Table S2. The cartesian coordinates for the optimized structure of reactant, transition state and product at IEFPCM/M06-2X/6-31++G(d,p) level of theory.

1. Tri

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.609794	3.442832	-0.020289
2	6	2.594080	2.490600	-0.026234
3	1	3.646138	2.743097	-0.033792
4	7	2.114125	1.269817	-0.021638
5	6	0.745041	1.426311	-0.011843
6	6	-0.306386	0.473086	-0.004388
7	8	-0.198118	-0.769222	-0.004938
8	7	-1.556420	1.070380	0.003585
9	1	-2.370123	0.421790	0.006503
10	6	-1.781419	2.431193	0.003520
11	7	-0.809654	3.331561	-0.003388
12	6	0.415458	2.775560	-0.011204
13	6	1.774960	4.889109	-0.022799
14	1	1.303773	5.311497	-0.911181
15	1	1.317044	5.313055	0.871765
16	1	2.840202	5.114203	-0.030941

17	7	-6.158167	-1.084175	0.023184
18	6	-6.022553	-2.434507	-0.047587
19	1	-6.944168	-3.005083	-0.061772
20	6	-4.802246	-3.022226	-0.096803
21	1	-4.696573	-4.096721	-0.152713
22	6	-3.665255	-2.151969	-0.068467
23	7	-2.426776	-2.652432	-0.107329
24	1	-1.622014	-2.026226	-0.075312
25	1	-2.279670	-3.648716	-0.153870
26	7	-3.800483	-0.823362	-0.002848
27	6	-5.033009	-0.259328	0.042404
28	8	-5.205643	0.969389	0.101757
29	6	-7.472884	-0.446544	0.079081
30	1	-7.557986	0.141708	0.993352
31	1	-7.600871	0.212143	-0.780664
32	1	-8.233673	-1.225113	0.066962
33	7	6.043472	-1.463419	0.014532
34	6	5.685278	-2.774888	0.055594
35	1	6.504402	-3.484293	0.077286
36	6	4.390590	-3.183966	0.068641
37	1	4.133712	-4.232981	0.100245
38	6	3.379162	-2.181211	0.038819
39	7	2.088095	-2.455882	0.048576
40	1	1.355045	-1.734429	0.025354

41	1	1.793563	-3.421774	0.078500
42	7	3.773514	-0.889988	-0.000917
43	6	5.086094	-0.461582	-0.011841
44	8	5.375053	0.723256	-0.042993
45	6	7.445882	-1.036857	0.000911
46	1	7.637582	-0.449192	-0.896997
47	1	7.650446	-0.428757	0.882462
48	1	8.074345	-1.924718	0.006109
49	1	3.065177	-0.088409	-0.013842
50	7	-3.062829	2.820474	0.006110
51	1	-3.839789	2.152397	0.043061
52	1	-3.246354	3.811800	0.025010

2. Tri-G(N2-H)•

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.632150	3.486905	-0.070891
2	6	2.574544	2.521783	-0.073318
3	1	3.635600	2.734479	-0.099958
4	7	2.061067	1.290402	-0.039493
5	6	0.726980	1.471694	-0.013169
6	6	-0.355105	0.511190	0.021522
7	8	-0.212613	-0.719700	0.029837
8	7	-1.576556	1.117422	0.041657
9	1	-2.396314	0.476014	0.055420
10	6	-1.828715	2.509471	0.029105

11	7	-3.028984	2.982647	0.059940
12	1	-3.734491	2.234367	0.102991
13	7	-0.778801	3.404080	-0.014926
14	6	0.409023	2.843947	-0.031398
15	6	1.825584	4.931972	-0.104565
16	1	1.349118	5.338409	-0.996803
17	1	1.383128	5.375374	0.787540
18	1	2.894352	5.135095	-0.129240
19	7	-6.156348	-1.061778	0.028752
20	6	-6.029712	-2.404540	-0.133380
21	1	-6.954817	-2.967435	-0.185171
22	6	-4.813084	-2.995750	-0.223796
23	1	-4.714318	-4.064623	-0.352820
24	6	-3.670994	-2.136001	-0.138292
25	7	-2.435278	-2.642647	-0.213061
26	1	-1.629819	-2.025536	-0.132471
27	1	-2.292888	-3.634453	-0.322895
28	7	-3.795491	-0.815266	0.017363
29	6	-5.025103	-0.244436	0.102742
30	8	-5.186248	0.976148	0.245124
31	6	-7.466086	-0.419810	0.128004
32	1	-7.549908	0.100434	1.082854
33	1	-7.585586	0.302060	-0.680799
34	1	-8.233449	-1.188691	0.055962

35	7	5.998625	-1.486146	0.030068
36	6	5.650608	-2.799517	0.092933
37	1	6.475651	-3.501631	0.124102
38	6	4.359468	-3.220960	0.115447
39	1	4.112284	-4.271588	0.164509
40	6	3.339258	-2.229596	0.072802
41	7	2.050008	-2.509600	0.092843
42	1	1.323320	-1.787133	0.062410
43	1	1.755207	-3.474660	0.140756
44	7	3.725810	-0.936122	0.009038
45	6	5.034878	-0.492732	-0.012181
46	8	5.308091	0.694216	-0.064575
47	6	7.398131	-1.048496	0.009643
48	1	7.585243	-0.475256	-0.898422
49	1	7.596547	-0.423972	0.880971
50	1	8.033121	-1.931340	0.030712
51	1	3.022720	-0.153812	-0.014362

3. Tri-G(N1-H)•

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.588685	3.238590	-0.000464
2	6	2.663936	2.429469	-0.000240
3	1	3.680958	2.800151	0.000038
4	7	2.346511	1.124517	-0.000327
5	6	1.009696	1.090239	-0.000625

6	6	0.064111	-0.028089	-0.000901
7	8	0.442153	-1.210206	-0.000969
8	7	-1.244703	0.328166	-0.001036
9	6	-1.609639	1.619018	-0.001033
10	7	-0.779486	2.743489	-0.000947
11	6	0.479278	2.409780	-0.000705
12	6	1.559883	4.697611	-0.000433
13	1	1.041370	5.046362	-0.893564
14	1	1.041334	5.046345	0.892686
15	1	2.585739	5.061562	-0.000410
16	7	-7.058101	-0.851608	0.001140
17	6	-6.770500	-2.179510	0.001010
18	1	-7.622120	-2.850729	0.001417
19	6	-5.491728	-2.631195	0.000382
20	1	-5.266915	-3.688993	0.000277
21	6	-4.458612	-1.637608	-0.000117
22	7	-3.168621	-1.992669	-0.000728
23	1	-2.446384	-1.267575	-0.001004
24	1	-2.905337	-2.965451	-0.000957
25	7	-4.742515	-0.334195	0.000011
26	6	-6.030178	0.102776	0.000672
27	8	-6.326601	1.302112	0.000857
28	6	-8.434987	-0.363328	0.001873
29	1	-8.610595	0.246023	0.889470

30	1	-8.611402	0.246367	-0.885324
31	1	-9.107368	-1.219770	0.002010
32	7	6.639075	-1.057752	0.001507
33	6	6.490245	-2.409897	-0.000014
34	1	7.411492	-2.980590	0.000049
35	6	5.277125	-3.020294	-0.001461
36	1	5.191334	-4.096962	-0.002580
37	6	4.118968	-2.191868	-0.001287
38	7	2.885692	-2.657952	-0.002209
39	1	2.057979	-2.046271	-0.001841
40	1	2.737199	-3.657596	-0.003067
41	7	4.310741	-0.853241	-0.000118
42	6	5.538362	-0.218358	0.001172
43	8	5.630606	0.997489	0.001983
44	6	7.959002	-0.419664	0.003224
45	1	8.064909	0.199795	-0.887539
46	1	8.061180	0.202156	0.892749
47	1	8.715123	-1.201702	0.005908
48	1	3.502208	-0.184514	-0.000223
49	7	-2.903928	1.899022	-0.001144
50	1	-3.599857	1.130029	-0.000927
51	1	-3.193336	2.867152	-0.001027

4. Int1

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	1.586370	3.380701	-0.199731
2	6	2.570303	2.427379	-0.178419
3	1	3.622481	2.679635	-0.194621
4	7	2.092546	1.206147	-0.138344
5	6	0.723389	1.362768	-0.122584
6	6	-0.331255	0.406325	-0.109719
7	8	-0.217605	-0.832424	-0.085598
8	7	-1.578961	1.004265	-0.125463
9	1	-2.394258	0.356667	-0.104451
10	6	-1.801712	2.364704	-0.146815
11	7	-3.078763	2.757081	-0.139143
12	1	-3.859285	2.090336	-0.142192
13	1	-3.259425	3.748876	-0.172170
14	7	-0.828654	3.268645	-0.177768
15	6	0.392207	2.717660	-0.169373
16	6	1.752560	4.826880	-0.232990
17	1	2.817750	5.050845	-0.253734
18	1	1.274498	5.230331	-1.126308
19	1	1.301149	5.267735	0.656699
20	7	-6.180328	-1.131860	-0.070677
21	6	-6.049674	-2.482704	-0.000599
22	1	-6.973478	-3.049523	0.019827
23	6	-4.831424	-3.075278	0.040715
24	1	-4.729687	-4.150169	0.096236

25	6	-3.691246	-2.209694	0.005073
26	7	-2.454699	-2.715340	0.037255
27	1	-1.647726	-2.093127	0.001133
28	1	-2.311102	-3.712149	0.083451
29	7	-3.821636	-0.880526	-0.060527
30	6	-5.052235	-0.311894	-0.097878
31	8	-5.220441	0.917678	-0.156548
32	6	-7.492904	-0.488924	-0.117811
33	1	-7.612154	0.170667	0.742474
34	1	-7.581941	0.099122	-1.031823
35	1	-8.256590	-1.264513	-0.099948
36	7	6.027056	-1.532731	-0.086325
37	6	5.671545	-2.844157	-0.026754
38	1	6.492182	-3.551726	-0.002413
39	6	4.377774	-3.255936	0.000640
40	1	4.123407	-4.305010	0.046821
41	6	3.364104	-2.256157	-0.034058
42	7	2.073582	-2.532320	-0.010564
43	1	1.341207	-1.811921	-0.040246
44	1	1.779707	-3.497911	0.032791
45	7	3.756339	-0.964887	-0.093690
46	6	5.068034	-0.533095	-0.119866
47	8	5.352880	0.651856	-0.169243
48	6	7.428676	-1.103818	-0.112686

49	1	7.615793	-0.530671	-1.020881
50	1	7.635196	-0.481083	0.758094
51	1	8.058638	-1.990423	-0.095118
52	1	3.049568	-0.168287	-0.113827
53	8	0.401597	1.581059	2.356918
54	1	1.243830	1.088372	2.389539

5. TS1

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.605110	3.332442	-0.183781
2	6	2.557283	2.375445	-0.159722
3	1	3.614112	2.600000	-0.231727
4	7	2.068726	1.144249	-0.056275
5	6	0.728499	1.313865	0.026592
6	6	-0.341906	0.357178	0.028738
7	8	-0.218123	-0.874740	0.079935
8	7	-1.580631	0.959108	-0.049031
9	1	-2.399655	0.313439	-0.060502
10	6	-1.788436	2.319739	-0.236358
11	7	-3.057212	2.690765	-0.411568
12	1	-3.833246	2.017238	-0.431496
13	1	-3.240499	3.677282	-0.518030
14	7	-0.820153	3.220903	-0.243881
15	6	0.391667	2.695053	0.024986
16	6	1.785457	4.774036	-0.160840

17	1	2.820543	5.001617	-0.410112
18	1	1.119784	5.229129	-0.894328
19	1	1.548465	5.147484	0.837863
20	7	-6.177662	-1.155114	-0.121622
21	6	-6.067647	-2.488895	0.114603
22	1	-6.998570	-3.041732	0.167382
23	6	-4.859507	-3.082596	0.272742
24	1	-4.773635	-4.143893	0.460130
25	6	-3.707779	-2.237483	0.178545
26	7	-2.480676	-2.748494	0.316657
27	1	-1.664791	-2.145116	0.235713
28	1	-2.352868	-3.734003	0.485979
29	7	-3.817633	-0.924365	-0.049092
30	6	-5.038887	-0.354835	-0.203627
31	8	-5.188166	0.859972	-0.418063
32	6	-7.478713	-0.509079	-0.293003
33	1	-7.612345	0.257704	0.470851
34	1	-7.531494	-0.043360	-1.277627
35	1	-8.254717	-1.266643	-0.198503
36	7	6.024497	-1.578443	-0.155768
37	6	5.684324	-2.893868	-0.097722
38	1	6.512358	-3.593001	-0.113627
39	6	4.396749	-3.319864	-0.023516
40	1	4.154685	-4.371846	0.022531

41	6	3.373277	-2.330684	-0.006050
42	7	2.086969	-2.618629	0.065197
43	1	1.354033	-1.902420	0.074918
44	1	1.799870	-3.586232	0.107038
45	7	3.750620	-1.035114	-0.066689
46	6	5.055766	-0.588318	-0.144076
47	8	5.324500	0.599905	-0.197951
48	6	7.419976	-1.135250	-0.231732
49	1	7.572599	-0.570168	-1.151450
50	1	7.646136	-0.501166	0.625704
51	1	8.059448	-2.015105	-0.223823
52	1	3.039253	-0.250042	-0.054391
53	8	0.559913	2.694913	2.025179
54	1	-0.278889	2.302619	2.318327

6. Int2

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.704379	3.336931	-0.046834
2	6	2.564649	2.332035	-0.133068
3	1	3.599056	2.463340	-0.430838
4	7	2.044771	1.126016	0.141580
5	6	0.756407	1.355981	0.457543
6	6	-0.318504	0.413819	0.437629
7	8	-0.201719	-0.820984	0.551541
8	7	-1.547715	1.004431	0.235689

9	1	-2.354494	0.358419	0.154241
10	6	-1.667467	2.305874	-0.262501
11	7	-2.869667	2.589190	-0.789550
12	1	-3.656456	1.934915	-0.734620
13	1	-3.044889	3.550293	-1.040938
14	7	-0.710257	3.194193	-0.257374
15	6	0.431344	2.821175	0.502120
16	6	1.970273	4.753141	-0.204412
17	1	2.962083	4.882171	-0.636628
18	1	1.220414	5.183809	-0.870221
19	1	1.927327	5.250378	0.767864
20	7	-6.101967	-1.187500	-0.343855
21	6	-6.001694	-2.515358	-0.072705
22	1	-6.925723	-3.080738	-0.113228
23	6	-4.811134	-3.089271	0.228702
24	1	-4.733406	-4.146054	0.443466
25	6	-3.667613	-2.227701	0.250087
26	7	-2.456781	-2.713804	0.542038
27	1	-1.648559	-2.093340	0.551773
28	1	-2.335105	-3.691576	0.754885
29	7	-3.767234	-0.922644	-0.018525
30	6	-4.969139	-0.372631	-0.321420
31	8	-5.105406	0.834304	-0.581332
32	6	-7.383988	-0.564472	-0.670036

33	1	-7.606014	0.221101	0.053014
34	1	-7.337930	-0.126303	-1.667708
35	1	-8.158060	-1.329176	-0.635847
36	7	5.868354	-1.698250	-0.439192
37	6	5.544837	-2.988019	-0.153460
38	1	6.357830	-3.701252	-0.223967
39	6	4.290786	-3.373366	0.197913
40	1	4.062989	-4.405964	0.419254
41	6	3.284582	-2.368261	0.264551
42	7	2.030643	-2.613367	0.595429
43	1	1.308287	-1.883984	0.610661
44	1	1.752922	-3.560233	0.812323
45	7	3.644139	-1.099496	-0.029509
46	6	4.916772	-0.693571	-0.380645
47	8	5.174245	0.474352	-0.621234
48	6	7.228890	-1.297923	-0.811132
49	1	7.215715	-0.844101	-1.802185
50	1	7.605931	-0.576103	-0.086360
51	1	7.857902	-2.185372	-0.815502
52	1	2.950346	-0.298411	0.031641
53	8	0.309817	3.264611	1.840620
54	1	-0.320323	4.001316	1.837878

7. TS2

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	1.661075	3.315289	-0.048173
2	6	2.528635	2.313359	-0.133412
3	1	3.569455	2.456921	-0.401907
4	7	2.010343	1.102382	0.105726
5	6	0.710912	1.311226	0.396106
6	6	-0.333529	0.327144	0.326783
7	8	-0.163277	-0.901549	0.408467
8	7	-1.598576	0.854750	0.133509
9	1	-2.416364	0.198900	0.107447
10	6	-1.764318	2.161799	-0.226150
11	7	-2.855956	2.835848	-0.463353
12	1	-3.742889	2.355592	-0.623764
13	1	-1.855921	3.752230	-0.555998
14	7	-0.737828	3.046164	-0.377433
15	6	0.383650	2.785942	0.455944
16	6	1.924632	4.735614	-0.180344
17	1	2.924183	4.872769	-0.591364
18	1	1.189458	5.174573	-0.857776
19	1	1.862156	5.220513	0.796884
20	7	-6.122133	-1.152645	-0.328318
21	6	-6.049327	-2.485977	-0.078559
22	1	-6.986546	-3.029403	-0.119054
23	6	-4.870212	-3.094756	0.202052
24	1	-4.816602	-4.156840	0.396867

25	6	-3.706788	-2.261439	0.224644
26	7	-2.501997	-2.778766	0.492867
27	1	-1.675116	-2.184998	0.479206
28	1	-2.397365	-3.764084	0.678082
29	7	-3.781403	-0.951200	-0.018701
30	6	-4.970949	-0.359075	-0.304495
31	8	-5.076896	0.850905	-0.544054
32	6	-7.392520	-0.495949	-0.632090
33	1	-7.592258	0.279586	0.108242
34	1	-7.343644	-0.038257	-1.620830
35	1	-8.183210	-1.243868	-0.607914
36	7	5.933897	-1.610634	-0.381643
37	6	5.644955	-2.910915	-0.106446
38	1	6.483327	-3.596220	-0.152012
39	6	4.394400	-3.338157	0.206630
40	1	4.193043	-4.377797	0.420372
41	6	3.353833	-2.367371	0.242165
42	7	2.098955	-2.653804	0.532383
43	1	1.355550	-1.946545	0.524308
44	1	1.844935	-3.609160	0.740821
45	7	3.680225	-1.086333	-0.038586
46	6	4.949287	-0.637420	-0.348935
47	8	5.175804	0.539265	-0.577234
48	6	7.291243	-1.165922	-0.712990

49	1	7.288866	-0.697077	-1.697022
50	1	7.630164	-0.445448	0.031756
51	1	7.944661	-2.035558	-0.715789
52	1	2.960078	-0.311483	0.005711
53	8	0.200019	3.210312	1.790674
54	1	-0.390792	3.978218	1.787541

8. Int3

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.738695	3.345236	-0.127464
2	6	2.584693	2.314033	-0.182961
3	1	3.632683	2.431271	-0.434670
4	7	2.032831	1.126811	0.070999
5	6	0.738866	1.376871	0.346716
6	6	-0.346276	0.439759	0.313108
7	8	-0.212969	-0.792864	0.424810
8	7	-1.576768	1.017039	0.129411
9	1	-2.388840	0.370771	0.124621
10	6	-1.804653	2.328939	-0.316007
11	7	-2.948439	2.807211	-0.599900
12	1	-3.691081	2.111775	-0.477531
13	1	-0.898255	4.085248	-0.666995
14	7	-0.657959	3.113506	-0.491263
15	6	0.450684	2.851822	0.377874
16	6	2.081711	4.753649	-0.227670

17	1	3.115309	4.834764	-0.562088
18	1	1.434239	5.244434	-0.956783
19	1	1.979910	5.236442	0.747314
20	7	-6.130107	-1.203804	-0.222839
21	6	-5.985620	-2.554294	-0.200005
22	1	-6.897778	-3.132273	-0.296880
23	6	-4.767980	-3.134928	-0.063928
24	1	-4.653821	-4.209962	-0.047003
25	6	-3.645030	-2.253986	0.054458
26	7	-2.408777	-2.747166	0.191408
27	1	-1.617493	-2.111925	0.278377
28	1	-2.254028	-3.742782	0.216618
29	7	-3.786891	-0.926793	0.033591
30	6	-5.016370	-0.365537	-0.104920
31	8	-5.192538	0.860207	-0.131308
32	6	-7.440614	-0.574380	-0.373872
33	1	-7.654025	0.048102	0.495946
34	1	-7.448052	0.050982	-1.267363
35	1	-8.191611	-1.357559	-0.463137
36	7	5.867665	-1.727939	-0.307256
37	6	5.532083	-3.012977	-0.013825
38	1	6.347854	-3.726158	-0.036910
39	6	4.264234	-3.394071	0.290068
40	1	4.027612	-4.422842	0.519517

41	6	3.255498	-2.389757	0.295101
42	7	1.987809	-2.627908	0.572844
43	1	1.270688	-1.894022	0.550061
44	1	1.697994	-3.570379	0.793060
45	7	3.628801	-1.125589	-0.003061
46	6	4.915544	-0.722712	-0.303693
47	8	5.182154	0.442138	-0.548236
48	6	7.243112	-1.333139	-0.627232
49	1	7.267882	-0.877398	-1.617072
50	1	7.596913	-0.614614	0.112474
51	1	7.867318	-2.223783	-0.611150
52	1	2.935807	-0.329004	0.016187
53	8	0.243465	3.282924	1.700927
54	1	-0.227429	4.129701	1.709310

9. Int2’

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.637600	3.186710	0.135727
2	6	2.540647	2.227958	-0.020977
3	1	3.562422	2.423518	-0.327301
4	7	2.080537	0.986668	0.194319
5	6	0.789349	1.139358	0.543073
6	6	-0.242237	0.151221	0.488837
7	8	-0.067603	-1.080184	0.534178
8	7	-1.502648	0.692954	0.338943

9	1	-2.279315	0.013349	0.232678
10	6	-1.698198	2.009885	-0.078464
11	7	-2.921375	2.280936	-0.546142
12	1	-3.658380	1.569653	-0.585182
13	1	-3.125937	3.245686	-0.783746
14	7	-0.770374	2.938441	-0.041014
15	6	0.402702	2.583686	0.678474
16	6	1.836072	4.620167	0.050897
17	1	2.824299	4.817181	-0.363080
18	1	1.075094	5.050425	-0.603283
19	1	1.760985	5.064977	1.046197
20	7	-5.939381	-1.690845	-0.367757
21	6	-5.788203	-3.012599	-0.090821
22	1	-6.686826	-3.616299	-0.145847
23	6	-4.579989	-3.535211	0.232780
24	1	-4.461619	-4.587456	0.451214
25	6	-3.473753	-2.626909	0.268687
26	7	-2.247571	-3.062590	0.575937
27	1	-1.463009	-2.412856	0.576406
28	1	-2.086269	-4.036363	0.780744
29	7	-3.624220	-1.326680	-0.000288
30	6	-4.843326	-0.828238	-0.323632
31	8	-5.027158	0.372061	-0.584561
32	6	-7.240599	-1.123502	-0.718966

33	1	-7.514638	-0.354290	0.003925
34	1	-7.191433	-0.676037	-1.712295
35	1	-7.979590	-1.922870	-0.708171
36	7	6.034913	-1.624091	-0.519150
37	6	5.780312	-2.935618	-0.264039
38	1	6.628534	-3.603658	-0.357450
39	6	4.550568	-3.393568	0.085984
40	1	4.376372	-4.441510	0.282092
41	6	3.494961	-2.443497	0.184550
42	7	2.258386	-2.761341	0.518606
43	1	1.499560	-2.071409	0.556650
44	1	2.032753	-3.726232	0.715720
45	7	3.786440	-1.150999	-0.080112
46	6	5.034337	-0.670900	-0.427015
47	8	5.230130	0.514828	-0.635987
48	6	7.370683	-1.146060	-0.889204
49	1	7.324555	-0.658243	-1.862910
50	1	7.721892	-0.433646	-0.142407
51	1	8.040302	-2.002234	-0.932296
52	1	3.054894	-0.388935	0.011942
53	8	0.288245	2.943791	2.041567
54	1	-0.375770	3.647610	2.098257
55	8	-2.215348	5.156587	-0.987753
56	1	-1.519712	4.589287	-0.594083

57	1	-2.371397	5.872513	-0.361790

10. TS2’

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.642858	3.207396	0.089015
2	6	2.548172	2.240354	-0.037912
3	1	3.578468	2.433210	-0.316053
4	7	2.079016	1.005508	0.173209
5	6	0.779971	1.160019	0.488495
6	6	-0.245463	0.163304	0.416624
7	8	-0.054964	-1.062264	0.466462
8	7	-1.517451	0.681544	0.249089
9	1	-2.296392	-0.007841	0.176567
10	6	-1.759084	1.979673	-0.151611
11	7	-2.943082	2.376539	-0.526095
12	1	-3.709426	1.696895	-0.543373
13	1	-2.916513	3.535241	-0.730837
14	7	-0.748112	2.887057	-0.180488
15	6	0.403971	2.610593	0.608748
16	6	1.862247	4.641388	0.019587
17	1	2.853783	4.824035	-0.392479
18	1	1.112822	5.092375	-0.634332
19	1	1.796459	5.079614	1.018325
20	7	-5.957665	-1.655012	-0.300925
21	6	-5.796842	-2.987652	-0.090897

22	1	-6.696738	-3.589764	-0.142873
23	6	-4.578155	-3.522725	0.166433
24	1	-4.451609	-4.583628	0.331743
25	6	-3.471743	-2.615334	0.206756
26	7	-2.236355	-3.064515	0.452260
27	1	-1.451406	-2.416646	0.463808
28	1	-2.070115	-4.046692	0.606680
29	7	-3.631199	-1.304390	0.003268
30	6	-4.861312	-0.791580	-0.255964
31	8	-5.054449	0.417453	-0.456018
32	6	-7.270056	-1.074642	-0.582252
33	1	-7.517663	-0.336147	0.180973
34	1	-7.255619	-0.586420	-1.557355
35	1	-8.008793	-1.874293	-0.578339
36	7	6.062745	-1.596883	-0.456455
37	6	5.814135	-2.910374	-0.205806
38	1	6.669515	-3.571240	-0.283524
39	6	4.582045	-3.379068	0.121760
40	1	4.413149	-4.428419	0.314843
41	6	3.516917	-2.438485	0.200501
42	7	2.276457	-2.764893	0.510803
43	1	1.515345	-2.078825	0.534127
44	1	2.051954	-3.730822	0.704122
45	7	3.803578	-1.143517	-0.058266

46	6	5.053538	-0.651816	-0.382405
47	8	5.241892	0.535613	-0.587037
48	6	7.401146	-1.108332	-0.803183
49	1	7.367042	-0.617702	-1.775922
50	1	7.735307	-0.396101	-0.048442
51	1	8.077009	-1.959919	-0.838364
52	1	3.067056	-0.391493	0.017121
53	8	0.234488	2.964396	1.961577
54	1	-0.325056	3.753232	2.019370
55	8	-2.298156	4.723025	-0.869114
56	1	-1.181608	3.893462	-0.414277
57	1	-2.599902	5.388330	-0.239626

11. Int3’

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.651942	3.220629	0.068916
2	6	2.561800	2.251695	-0.053254
3	1	3.599592	2.451855	-0.295725
4	7	2.086966	1.016651	0.121053
5	6	0.780751	1.165791	0.411415
6	6	-0.247364	0.170826	0.322526
7	8	-0.046863	-1.056293	0.362883
8	7	-1.511767	0.687841	0.171102
9	1	-2.287100	-0.001675	0.131622
10	6	-1.807938	2.002702	-0.207160

11	7	-2.983628	2.414688	-0.492402
12	1	-3.689576	1.674790	-0.430997
13	1	-2.974616	4.244585	-0.752863
14	7	-0.722831	2.870054	-0.307454
15	6	0.400886	2.613145	0.539413
16	6	1.894602	4.653741	0.068220
17	1	2.904175	4.834343	-0.298591
18	1	1.182545	5.149929	-0.594438
19	1	1.800895	5.052228	1.081370
20	7	-5.955247	-1.749458	-0.190244
21	6	-5.748878	-3.090818	-0.132157
22	1	-6.635246	-3.711837	-0.194674
23	6	-4.503655	-3.611467	-0.003894
24	1	-4.340316	-4.679244	0.041134
25	6	-3.420166	-2.677867	0.068619
26	7	-2.160855	-3.111043	0.197227
27	1	-1.397132	-2.439747	0.251424
28	1	-1.961332	-4.097615	0.250627
29	7	-3.622688	-1.359467	0.011058
30	6	-4.878914	-0.859350	-0.120759
31	8	-5.112060	0.355919	-0.181759
32	6	-7.295969	-1.184407	-0.331760
33	1	-7.513113	-0.533721	0.516098
34	1	-7.355076	-0.600272	-1.250953

35	1	-8.013780	-2.002361	-0.365175
36	7	6.086584	-1.596372	-0.371629
37	6	5.826137	-2.907850	-0.122064
38	1	6.681846	-3.571289	-0.168584
39	6	4.582870	-3.371242	0.168180
40	1	4.404443	-4.419021	0.361437
41	6	3.518195	-2.427342	0.206942
42	7	2.267296	-2.747899	0.477563
43	1	1.507101	-2.058597	0.473075
44	1	2.033985	-3.712113	0.669138
45	7	3.817248	-1.134397	-0.048983
46	6	5.078514	-0.647867	-0.334420
47	8	5.277263	0.538082	-0.537924
48	6	7.436854	-1.114201	-0.678571
49	1	7.434178	-0.625479	-1.652862
50	1	7.751570	-0.401887	0.084447
51	1	8.109475	-1.968967	-0.691965
52	1	3.080504	-0.380419	-0.001235
53	8	0.172761	2.941163	1.888706
54	1	-0.346166	3.756951	1.949975
55	8	-2.518438	5.110679	-0.870481
56	1	-1.012087	3.840881	-0.453907
57	1	-2.883569	5.710740	-0.210894

12. Int4

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	7	1.696349	3.142391	-0.199620
2	6	2.571777	2.136273	-0.237044
3	1	3.617156	2.278125	-0.486934
4	7	2.051995	0.938675	0.042217
5	6	0.746337	1.156561	0.295147
6	6	-0.311502	0.186302	0.259571
7	8	-0.145751	-1.039402	0.398793
8	7	-1.550760	0.725946	0.039257
9	1	-2.347315	0.060915	0.043783
10	6	-1.807652	2.031094	-0.416374
11	7	-2.966833	2.474063	-0.697641
12	1	-3.688979	1.761141	-0.556167
13	1	-0.963819	3.829615	-0.664923
14	7	-0.685199	2.847092	-0.606454
15	6	0.413055	2.621075	0.277401
16	6	1.958480	4.557108	-0.405023
17	1	2.997005	4.675697	-0.711717
18	1	1.300478	4.943156	-1.186098
19	1	1.781446	5.106879	0.521558
20	7	-6.055934	-1.606369	-0.195099
21	6	-5.879416	-2.952350	-0.147124
22	1	-6.779431	-3.553103	-0.213749
23	6	-4.646108	-3.501875	-0.022876

24	1	-4.506580	-4.573333	0.014697
25	6	-3.542162	-2.593031	0.056224
26	7	-2.292336	-3.054375	0.181743
27	1	-1.516030	-2.398920	0.251969
28	1	-2.114354	-4.045258	0.230520
29	7	-3.715289	-1.270411	0.008445
30	6	-4.959826	-0.740329	-0.118508
31	8	-5.164653	0.480047	-0.168941
32	6	-7.383551	-1.010535	-0.332245
33	1	-7.590911	-0.369504	0.525453
34	1	-7.425882	-0.409948	-1.241642
35	1	-8.118510	-1.812220	-0.382662
36	7	5.964082	-1.826617	-0.267808
37	6	5.656387	-3.115182	0.040629
38	1	6.488297	-3.809789	0.031001
39	6	4.395895	-3.521221	0.342643
40	1	4.180713	-4.552172	0.583463
41	6	3.364380	-2.540341	0.328411
42	7	2.100972	-2.804002	0.602192
43	1	1.366103	-2.088424	0.561721
44	1	1.832005	-3.749623	0.834825
45	7	3.710275	-1.271777	0.015813
46	6	4.989119	-0.843574	-0.283451
47	8	5.230289	0.323679	-0.542509

48	6	7.331778	-1.404683	-0.586501
49	1	7.352129	-0.965638	-1.583990
50	1	7.663626	-0.665283	0.142715
51	1	7.976864	-2.279760	-0.551048
52	1	2.998421	-0.491969	0.019745
53	8	0.088856	3.185292	1.536616
54	1	0.760762	2.950516	2.194883
55	8	-0.986005	5.573883	0.410948
56	1	-0.818153	5.064941	1.218089
57	1	-1.810101	6.051885	0.558664

13. TS3

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.628274	3.139880	-0.558038
2	6	2.580414	2.174934	-0.422328
3	1	3.639550	2.392034	-0.471020
4	7	2.070605	0.967441	-0.226048
5	6	0.731426	1.147750	-0.218297
6	6	-0.348862	0.182922	-0.144327
7	8	-0.184635	-1.032609	0.007359
8	7	-1.584719	0.745313	-0.288431
9	1	-2.389537	0.089935	-0.197590
10	6	-1.896906	2.107865	-0.455961
11	7	-3.067252	2.595183	-0.439105
12	1	-3.778812	1.878210	-0.262087

13	1	-1.020763	3.947197	-0.513188
14	7	-0.807686	2.964629	-0.698813
15	6	0.424573	2.517654	-0.365204
16	6	1.835551	4.568949	-0.775961
17	1	2.899389	4.735343	-0.934184
18	1	1.283335	4.878601	-1.664749
19	1	1.486436	5.125129	0.094849
20	7	-6.109952	-1.489153	0.063664
21	6	-5.964702	-2.836820	-0.022773
22	1	-6.880739	-3.416500	-0.009237
23	6	-4.741179	-3.413103	-0.117867
24	1	-4.626925	-4.486110	-0.183964
25	6	-3.612934	-2.531739	-0.119274
26	7	-2.370982	-3.023037	-0.200998
27	1	-1.574747	-2.392101	-0.152953
28	1	-2.214332	-4.017901	-0.243199
29	7	-3.755503	-1.206259	-0.041322
30	6	-4.991970	-0.649710	0.049592
31	8	-5.170470	0.573919	0.122258
32	6	-7.427247	-0.863976	0.168598
33	1	-7.483510	-0.276756	1.085770
34	1	-7.593172	-0.205472	-0.684935
35	1	-8.181368	-1.649019	0.184092
36	7	6.033921	-1.763883	0.073813

37	6	5.697547	-3.074924	0.206684
38	1	6.528861	-3.766735	0.276361
39	6	4.410202	-3.506650	0.250055
40	1	4.172112	-4.555327	0.354359
41	6	3.381736	-2.528153	0.153767
42	7	2.094680	-2.816707	0.190231
43	1	1.365128	-2.101512	0.121154
44	1	1.805819	-3.779062	0.294622
45	7	3.756771	-1.237035	0.017624
46	6	5.061768	-0.783565	-0.032198
47	8	5.323739	0.400104	-0.159459
48	6	7.429714	-1.315782	0.036293
49	1	7.623220	-0.808481	-0.908967
50	1	7.611902	-0.627869	0.862114
51	1	8.071588	-2.188946	0.129798
52	1	3.046784	-0.466736	-0.058285
53	8	0.175236	2.534821	1.710205
54	1	1.034114	2.350005	2.122274
55	8	-0.614600	5.073438	1.199084
56	1	-0.352540	4.212733	1.599940
57	1	-1.337856	5.423438	1.730614

14. Int5

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.630378	3.147707	-0.716832

2	6	2.576442	2.151538	-0.573256
3	1	3.633961	2.346206	-0.694307
4	7	2.050987	0.985485	-0.293763
5	6	0.701595	1.216227	-0.174282
6	6	-0.396773	0.264491	-0.163835
7	8	-0.259009	-0.959172	-0.074570
8	7	-1.626986	0.853443	-0.268781
9	1	-2.443937	0.211824	-0.191835
10	6	-1.911900	2.224292	-0.351287
11	7	-3.062264	2.753296	-0.288822
12	1	-3.796016	2.052753	-0.136281
13	1	-0.984905	4.055559	-0.590470
14	7	-0.799907	3.058656	-0.562934
15	6	0.437238	2.557969	-0.505489
16	6	1.864794	4.556431	-1.024146
17	1	2.934204	4.695613	-1.171663
18	1	1.336457	4.820464	-1.941523
19	1	1.518822	5.157705	-0.182533
20	7	-6.199656	-1.281160	0.045681
21	6	-6.083711	-2.629713	-0.068437
22	1	-7.012118	-3.189538	-0.065271
23	6	-4.873234	-3.230523	-0.177530
24	1	-4.782885	-4.304173	-0.266716
25	6	-3.725975	-2.373975	-0.163687

26	7	-2.495028	-2.889719	-0.257974
27	1	-1.684737	-2.276284	-0.210309
28	1	-2.359976	-3.886384	-0.324573
29	7	-3.840013	-1.047624	-0.057830
30	6	-5.063647	-0.466238	0.047521
31	8	-5.215511	0.759251	0.146971
32	6	-7.502912	-0.629671	0.165626
33	1	-7.547785	-0.065454	1.097786
34	1	-7.652511	0.054409	-0.670598
35	1	-8.274399	-1.397780	0.159622
36	7	5.943945	-1.819497	0.038649
37	6	5.575846	-3.118789	0.198411
38	1	6.389937	-3.829093	0.284034
39	6	4.278279	-3.517755	0.248457
40	1	4.015133	-4.558104	0.373336
41	6	3.274143	-2.516416	0.129906
42	7	1.980264	-2.773594	0.169236
43	1	1.267160	-2.043599	0.077941
44	1	1.668868	-3.726619	0.293362
45	7	3.679940	-1.237739	-0.031333
46	6	4.995531	-0.818624	-0.091337
47	8	5.287919	0.354700	-0.246836
48	6	7.350141	-1.406651	-0.006929
49	1	7.560697	-0.936503	-0.967702

50	1	7.545011	-0.695664	0.796073
51	1	7.970111	-2.291362	0.119968
52	1	2.986591	-0.448107	-0.118289
53	8	0.371042	1.627972	1.879834
54	1	1.184314	1.189773	2.178524
55	8	0.591004	4.353619	1.835776
56	1	0.498180	3.382043	1.967723
57	1	0.019514	4.771016	2.489001

15. Int6

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.614371	3.138374	-0.718462
2	6	2.569589	2.146045	-0.588462
3	1	3.625190	2.352334	-0.707987
4	7	2.055084	0.973338	-0.327941
5	6	0.707316	1.194010	-0.200271
6	6	-0.384360	0.239361	-0.176486
7	8	-0.242430	-0.984496	-0.086639
8	7	-1.621217	0.824688	-0.246669
9	1	-2.434068	0.175400	-0.168334
10	6	-1.916640	2.193445	-0.353143
11	7	-3.068732	2.715755	-0.272069
12	1	-3.793503	2.013532	-0.087588
13	1	-0.992309	4.026636	-0.546144
14	7	-0.813357	3.028355	-0.601241

15	6	0.426872	2.535560	-0.517913
16	6	1.836634	4.547858	-1.031630
17	1	2.909817	4.710408	-1.112128
18	1	1.359976	4.789026	-1.983087
19	1	1.423633	5.153081	-0.223853
20	7	-6.172628	-1.322173	0.072103
21	6	-6.059726	-2.662804	-0.115190
22	1	-6.988491	-3.221768	-0.130484
23	6	-4.851420	-3.257785	-0.270943
24	1	-4.763561	-4.325277	-0.417902
25	6	-3.702971	-2.404158	-0.226197
26	7	-2.474024	-2.915090	-0.362562
27	1	-1.662412	-2.306606	-0.287467
28	1	-2.341248	-3.907207	-0.481107
29	7	-3.814245	-1.085095	-0.049174
30	6	-5.035762	-0.509475	0.103568
31	8	-5.183921	0.708955	0.271492
32	6	-7.473377	-0.676379	0.241481
33	1	-7.509156	-0.168010	1.205631
34	1	-7.627689	0.056159	-0.551708
35	1	-8.246991	-1.441039	0.196289
36	7	5.973124	-1.785120	0.082806
37	6	5.615269	-3.085979	0.252601
38	1	6.434827	-3.788090	0.352247

39	6	4.320885	-3.495875	0.295629
40	1	4.065631	-4.537209	0.428671
41	6	3.309281	-2.504482	0.158272
42	7	2.017469	-2.773602	0.188124
43	1	1.298482	-2.051659	0.083931
44	1	1.713832	-3.728095	0.319436
45	7	3.704672	-1.223836	-0.011493
46	6	5.017035	-0.794034	-0.065777
47	8	5.300768	0.379920	-0.232224
48	6	7.375973	-1.360506	0.043586
49	1	7.590594	-0.900931	-0.921414
50	1	7.557786	-0.637505	0.838860
51	1	8.002608	-2.237976	0.187162
52	1	3.004335	-0.441379	-0.116744
53	8	0.609145	1.795364	1.899761
54	1	-0.139227	1.267430	2.223911
55	8	0.079600	4.470905	1.655554
56	1	0.259413	3.528659	1.878725
57	1	0.416023	4.996933	2.388822

16. TS4

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.602370	3.136852	-0.606063
2	6	2.550656	2.184936	-0.428614
3	1	3.610224	2.405745	-0.445344

4	7	2.044020	0.962327	-0.250443
5	6	0.719196	1.130418	-0.287069
6	6	-0.359250	0.157103	-0.187182
7	8	-0.183440	-1.052427	-0.028451
8	7	-1.595439	0.721941	-0.305988
9	1	-2.403083	0.062142	-0.213293
10	6	-1.904599	2.086850	-0.447863
11	7	-3.072128	2.579157	-0.406371
12	1	-3.787137	1.861830	-0.228508
13	1	-0.992141	3.945316	-0.271644
14	7	-0.824586	2.968479	-0.659060
15	6	0.403443	2.499426	-0.481265
16	6	1.812070	4.575302	-0.759204
17	1	2.860198	4.738225	-1.001860
18	1	1.186405	4.937142	-1.575730
19	1	1.542899	5.077818	0.170096
20	7	-6.103933	-1.474599	0.081584
21	6	-5.969522	-2.823923	0.002620
22	1	-6.889636	-3.396606	0.028591
23	6	-4.751253	-3.409668	-0.100048
24	1	-4.645362	-4.483892	-0.159897
25	6	-3.616349	-2.537605	-0.117438
26	7	-2.379956	-3.040075	-0.206203
27	1	-1.577329	-2.417746	-0.167744

28	1	-2.232459	-4.036639	-0.241594
29	7	-3.748861	-1.209810	-0.048164
30	6	-4.980824	-0.644746	0.051122
31	8	-5.149715	0.581182	0.117615
32	6	-7.415664	-0.838648	0.195365
33	1	-7.457760	-0.244413	1.108688
34	1	-7.585379	-0.185529	-0.661494
35	1	-8.175040	-1.618128	0.224622
36	7	6.033687	-1.749950	0.083013
37	6	5.714355	-3.065709	0.211272
38	1	6.554833	-3.746147	0.282468
39	6	4.432911	-3.515997	0.247921
40	1	4.209193	-4.568186	0.348235
41	6	3.391394	-2.552378	0.149141
42	7	2.107963	-2.857376	0.176066
43	1	1.372540	-2.150738	0.101695
44	1	1.829002	-3.823214	0.274957
45	7	3.750516	-1.255798	0.020279
46	6	5.049353	-0.782546	-0.023696
47	8	5.293109	0.405093	-0.146641
48	6	7.423674	-1.282928	0.050751
49	1	7.612509	-0.770162	-0.892479
50	1	7.594148	-0.595353	0.879301
51	1	8.076962	-2.147694	0.143094

52	1	3.034797	-0.499412	-0.058959
53	8	0.502322	2.895570	1.892021
54	1	-0.033864	2.298913	2.430092
55	8	-0.680259	4.874695	1.063999
56	1	-0.204501	4.026720	1.557646
57	1	-1.449294	5.149752	1.575297

17. Int7

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.611053	3.088396	-0.653871
2	6	2.556009	2.145560	-0.477934
3	1	3.615432	2.367006	-0.467306
4	7	2.051147	0.917255	-0.328334
5	6	0.718998	1.081558	-0.398180
6	6	-0.358371	0.122741	-0.273918
7	8	-0.207639	-1.095288	-0.106007
8	7	-1.585141	0.713678	-0.359186
9	1	-2.400489	0.073746	-0.260997
10	6	-1.847162	2.092480	-0.524922
11	7	-3.044323	2.566736	-0.549454
12	1	-3.751880	1.827258	-0.441700
13	1	-1.124273	4.613734	0.504159
14	7	-0.796854	2.982494	-0.660527
15	6	0.395143	2.440600	-0.590740
16	6	1.791895	4.531372	-0.750154

17	1	2.850357	4.737625	-0.897786
18	1	1.219631	4.905243	-1.599285
19	1	1.439794	4.999826	0.170998
20	7	-6.147277	-1.470914	0.012206
21	6	-6.009025	-2.804846	0.228754
22	1	-6.929324	-3.369618	0.326067
23	6	-4.787188	-3.385479	0.316552
24	1	-4.679015	-4.447237	0.489431
25	6	-3.652467	-2.524336	0.169381
26	7	-2.412577	-3.020888	0.241476
27	1	-1.612481	-2.401928	0.129067
28	1	-2.262040	-4.005155	0.398115
29	7	-3.788161	-1.212506	-0.042627
30	6	-5.022862	-0.652339	-0.125327
31	8	-5.194860	0.559742	-0.318550
32	6	-7.462743	-0.840154	-0.083968
33	1	-7.567774	-0.084914	0.695871
34	1	-7.571446	-0.361561	-1.057877
35	1	-8.223937	-1.608791	0.038477
36	7	6.014881	-1.798073	0.040671
37	6	5.676540	-3.109980	0.160239
38	1	6.506605	-3.802371	0.238601
39	6	4.388700	-3.541585	0.181020
40	1	4.149115	-4.590902	0.275100

41	6	3.361726	-2.562174	0.074139
42	7	2.074461	-2.851781	0.087827
43	1	1.343010	-2.137669	0.011560
44	1	1.786180	-3.815610	0.179301
45	7	3.738568	-1.270132	-0.046857
46	6	5.044100	-0.816915	-0.072071
47	8	5.308627	0.367775	-0.185228
48	6	7.410960	-1.349702	0.025149
49	1	7.613966	-0.827472	-0.909900
50	1	7.584985	-0.674858	0.863488
51	1	8.052072	-2.224227	0.110959
52	1	3.028494	-0.498118	-0.136551
53	8	0.953760	3.094162	2.219232
54	1	0.628797	2.542031	2.938575
55	8	-0.811854	5.086062	1.295139
56	1	0.278749	3.785120	2.085971
57	1	-1.594755	5.428573	1.741574

18. Int8

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.572596	3.384177	-0.248802
2	6	2.555086	2.426236	-0.249159
3	1	3.605365	2.676759	-0.325079
4	7	2.082807	1.206562	-0.154988
5	6	0.719352	1.364705	-0.044214

6	6	-0.338992	0.400620	-0.091276
7	8	-0.215052	-0.832516	-0.119566
8	7	-1.585796	0.995174	-0.103102
9	1	-2.402049	0.345971	-0.097860
10	6	-1.807630	2.354836	-0.094610
11	7	-3.077710	2.749819	-0.058223
12	1	-3.861102	2.083942	-0.023203
13	1	-3.255606	3.743160	-0.070676
14	7	-0.833848	3.267127	-0.141910
15	6	0.382134	2.727134	-0.148005
16	6	1.739669	4.828028	-0.343800
17	1	1.209676	5.199588	-1.221464
18	1	1.343179	5.302177	0.554749
19	1	2.802094	5.046337	-0.436472
20	7	-6.177189	-1.122597	-0.017201
21	6	-6.053878	-2.474555	-0.080277
22	1	-6.980321	-3.037371	-0.076425
23	6	-4.839359	-3.072914	-0.143373
24	1	-4.743470	-4.148628	-0.192871
25	6	-3.695024	-2.212523	-0.137787
26	7	-2.461685	-2.724018	-0.190640
27	1	-1.651649	-2.106148	-0.173390
28	1	-2.322935	-3.721805	-0.230140
29	7	-3.818642	-0.882201	-0.080269

30	6	-5.045641	-0.308167	-0.021059
31	8	-5.207001	0.923051	0.031435
32	6	-7.485640	-0.473223	0.054930
33	1	-7.549827	0.123934	0.965054
34	1	-7.622625	0.178430	-0.808743
35	1	-8.252779	-1.245506	0.063208
36	7	6.035794	-1.513527	-0.033743
37	6	5.688022	-2.825090	0.058233
38	1	6.512862	-3.526240	0.109932
39	6	4.396705	-3.245046	0.083781
40	1	4.148541	-4.294187	0.155190
41	6	3.377330	-2.253553	0.012670
42	7	2.088250	-2.536826	0.034004
43	1	1.354468	-1.821628	-0.024986
44	1	1.798388	-3.501893	0.105663
45	7	3.762028	-0.962068	-0.081212
46	6	5.071168	-0.521654	-0.107141
47	8	5.347920	0.663255	-0.188951
48	6	7.435005	-1.076235	-0.054506
49	1	7.630179	-0.527705	-0.976095
50	1	7.626261	-0.427995	0.801004
51	1	8.070037	-1.957933	-0.003731
52	1	3.051771	-0.172928	-0.117713
53	8	0.393525	1.483805	2.161636

54	1	1.238349	1.025960	2.313778

19. TS5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.556757	3.367938	-0.320725
2	6	2.530670	2.401816	-0.299838
3	1	3.573802	2.632910	-0.475058
4	7	2.063420	1.198488	-0.071117
5	6	0.710302	1.378173	0.168664
6	6	-0.352366	0.407087	0.006589
7	8	-0.211919	-0.819252	-0.072058
8	7	-1.596766	0.994220	-0.030995
9	1	-2.413260	0.343369	-0.059486
10	6	-1.818641	2.356122	-0.030294
11	7	-3.086504	2.751124	0.017170
12	1	-3.868355	2.084042	0.078722
13	1	-3.266308	3.743912	-0.017513
14	7	-0.843661	3.266431	-0.116263
15	6	0.370991	2.733598	-0.100737
16	6	1.721824	4.790753	-0.584685
17	1	1.119736	5.071725	-1.449571
18	1	1.405443	5.364864	0.287011
19	1	2.773244	4.984131	-0.790415
20	7	-6.171569	-1.121143	-0.018033
21	6	-6.050954	-2.464947	-0.181914

22	1	-6.977900	-3.026271	-0.208438
23	6	-4.838175	-3.058073	-0.303206
24	1	-4.744786	-4.127347	-0.432609
25	6	-3.692411	-2.201821	-0.246292
26	7	-2.460428	-2.709388	-0.348005
27	1	-1.649065	-2.098178	-0.276117
28	1	-2.323547	-3.702797	-0.451908
29	7	-3.813828	-0.879071	-0.091772
30	6	-5.039072	-0.309801	0.023633
31	8	-5.196988	0.914703	0.167432
32	6	-7.477933	-0.476707	0.115351
33	1	-7.533960	0.046191	1.070622
34	1	-7.618569	0.241998	-0.692703
35	1	-8.247298	-1.245303	0.067312
36	7	6.029403	-1.497647	-0.045408
37	6	5.689834	-2.810097	0.061578
38	1	6.518940	-3.507165	0.098053
39	6	4.401253	-3.235605	0.118079
40	1	4.158928	-4.285364	0.199802
41	6	3.376763	-2.248549	0.064084
42	7	2.089221	-2.536203	0.113530
43	1	1.354949	-1.822657	0.055490
44	1	1.802735	-3.501460	0.194680
45	7	3.752855	-0.955809	-0.042481

46	6	5.058823	-0.510473	-0.104839
47	8	5.328760	0.674739	-0.204505
48	6	7.425895	-1.054803	-0.099287
49	1	7.603561	-0.524533	-1.035080
50	1	7.627957	-0.388325	0.739467
51	1	8.065650	-1.932576	-0.040376
52	1	3.036309	-0.169075	-0.055972
53	8	0.525462	1.429303	2.100204
54	1	1.306157	0.889362	2.302884

20. Int9

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.482348	3.296847	-0.474684
2	6	2.418299	2.307986	-0.445509
3	1	3.395832	2.442434	-0.895349
4	7	2.032875	1.202896	0.135293
5	6	0.722773	1.473442	0.687995
6	6	-0.359221	0.473616	0.358823
7	8	-0.165297	-0.745494	0.231866
8	7	-1.603511	1.022178	0.264281
9	1	-2.398607	0.353011	0.164496
10	6	-1.854372	2.385724	0.185870
11	7	-3.140572	2.763450	0.275394
12	1	-3.899615	2.074963	0.300951
13	1	-3.351228	3.730566	0.079294

14	7	-0.889113	3.272366	-0.012576
15	6	0.337541	2.778958	0.088631
16	6	1.566804	4.568435	-1.173084
17	1	0.866027	4.578929	-2.010718
18	1	1.325008	5.380856	-0.486297
19	1	2.583698	4.694359	-1.542131
20	7	-6.098287	-1.202978	-0.209243
21	6	-5.920391	-2.506305	-0.550524
22	1	-6.823459	-3.079788	-0.725562
23	6	-4.682428	-3.047553	-0.662188
24	1	-4.543281	-4.085042	-0.932634
25	6	-3.573730	-2.180699	-0.400290
26	7	-2.320164	-2.637955	-0.481335
27	1	-1.537542	-2.022970	-0.264046
28	1	-2.141763	-3.601137	-0.719626
29	7	-3.750962	-0.897921	-0.069236
30	6	-4.999706	-0.377428	0.030366
31	8	-5.207321	0.810027	0.328701
32	6	-7.431706	-0.614041	-0.090766
33	1	-7.570850	-0.220004	0.916395
34	1	-7.540702	0.199605	-0.808848
35	1	-8.169789	-1.388521	-0.291844
36	7	5.955135	-1.477277	-0.237617
37	6	5.654651	-2.763032	0.086947

38	1	6.489205	-3.454582	0.083319
39	6	4.395356	-3.169429	0.393081
40	1	4.181766	-4.199074	0.641182
41	6	3.362179	-2.189998	0.365983
42	7	2.097300	-2.461393	0.634229
43	1	1.353401	-1.761616	0.540456
44	1	1.833410	-3.407131	0.871129
45	7	3.698787	-0.921459	0.050668
46	6	4.973695	-0.498249	-0.264574
47	8	5.214762	0.664162	-0.547835
48	6	7.319034	-1.054099	-0.568470
49	1	7.336009	-0.639049	-1.576369
50	1	7.646578	-0.294492	0.141667
51	1	7.970797	-1.923196	-0.512058
52	1	2.974587	-0.122826	0.092266
53	8	0.783012	1.608935	2.121830
54	1	1.199748	0.808412	2.477864

21. TS6

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.483730	3.289272	-0.414237
2	6	2.400356	2.287318	-0.415684
3	1	3.385691	2.421510	-0.848231
4	7	1.996824	1.170761	0.134466
5	6	0.688341	1.432338	0.695314

6	6	-0.386089	0.417255	0.308458
7	8	-0.155661	-0.787615	0.182652
8	7	-1.651787	0.919409	0.184267
9	1	-2.452175	0.234824	0.096996
10	6	-1.906426	2.265032	0.147285
11	7	-3.018374	2.946610	0.227268
12	1	-3.920208	2.470482	0.219443
13	1	-2.011435	3.901406	0.067989
14	7	-0.921961	3.182952	-0.022028
15	6	0.348256	2.793390	0.189425
16	6	1.592434	4.592934	-1.046231
17	1	0.811449	4.696920	-1.803065
18	1	1.484524	5.380395	-0.298390
19	1	2.570765	4.669212	-1.518501
20	7	-6.114814	-1.134970	-0.207225
21	6	-5.984417	-2.459920	-0.477343
22	1	-6.907977	-3.008712	-0.623004
23	6	-4.767965	-3.054483	-0.558007
24	1	-4.669701	-4.109553	-0.772545
25	6	-3.627629	-2.217127	-0.343359
26	7	-2.389560	-2.720795	-0.403943
27	1	-1.584802	-2.121913	-0.234979
28	1	-2.242215	-3.697694	-0.604291
29	7	-3.759157	-0.915486	-0.076461

30	6	-4.986782	-0.334897	-0.005173
31	8	-5.143571	0.869573	0.231945
32	6	-7.425372	-0.491961	-0.122692
33	1	-7.551340	-0.043123	0.863150
34	1	-7.502722	0.288688	-0.880492
35	1	-8.192172	-1.246875	-0.287471
36	7	5.974043	-1.429193	-0.244259
37	6	5.697649	-2.725853	0.056555
38	1	6.547036	-3.399075	0.052655
39	6	4.443711	-3.163637	0.340773
40	1	4.248323	-4.201342	0.569537
41	6	3.391030	-2.205806	0.316473
42	7	2.128739	-2.508245	0.563643
43	1	1.375889	-1.820476	0.473974
44	1	1.879716	-3.462238	0.782757
45	7	3.703345	-0.925075	0.026653
46	6	4.972883	-0.470260	-0.266586
47	8	5.193372	0.701221	-0.528043
48	6	7.332365	-0.973281	-0.554163
49	1	7.349035	-0.535493	-1.552356
50	1	7.640498	-0.224011	0.175426
51	1	7.999231	-1.831675	-0.512269
52	1	2.960895	-0.144188	0.074238
53	8	0.724004	1.452747	2.132956

54	1	1.125279	0.622601	2.436070

22. Int10

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.468128	3.273882	-0.574493
2	6	2.356953	2.249088	-0.525464
3	1	3.303681	2.295814	-1.053851
4	7	1.987502	1.232025	0.199475
5	6	0.718564	1.586819	0.810524
6	6	-0.388381	0.582315	0.488100
7	8	-0.176383	-0.633186	0.488022
8	7	-1.616817	1.098906	0.261894
9	1	-2.392762	0.407040	0.169051
10	6	-1.965219	2.461650	0.177049
11	7	-3.158078	2.906017	0.181272
12	1	-3.843281	2.150186	0.274221
13	1	-1.144203	4.308707	-0.025137
14	7	-0.894316	3.328018	0.037452
15	6	0.403962	2.930100	0.244544
16	6	1.580622	4.504229	-1.338629
17	1	0.731845	4.591099	-2.021270
18	1	1.604258	5.364447	-0.666692
19	1	2.503178	4.469608	-1.916255
20	7	-6.014869	-1.283140	-0.279150
21	6	-5.786153	-2.557728	-0.688950

22	1	-6.665106	-3.145622	-0.928144
23	6	-4.529180	-3.056806	-0.787823
24	1	-4.349470	-4.072464	-1.111784
25	6	-3.457757	-2.174511	-0.437345
26	7	-2.187512	-2.591279	-0.500614
27	1	-1.438810	-1.973867	-0.196212
28	1	-1.970597	-3.536800	-0.774399
29	7	-3.682342	-0.919602	-0.040913
30	6	-4.950263	-0.438207	0.049439
31	8	-5.200596	0.719005	0.412128
32	6	-7.368703	-0.742355	-0.171340
33	1	-7.554889	-0.418785	0.853290
34	1	-7.479018	0.113116	-0.838900
35	1	-8.075380	-1.522810	-0.448132
36	7	5.836117	-1.536692	-0.318627
37	6	5.545979	-2.809865	0.059386
38	1	6.371286	-3.511180	0.017554
39	6	4.306644	-3.193961	0.461615
40	1	4.101459	-4.214403	0.750886
41	6	3.284248	-2.204216	0.481334
42	7	2.038538	-2.451210	0.845032
43	1	1.306490	-1.738924	0.784351
44	1	1.776998	-3.384981	1.127706
45	7	3.610626	-0.948344	0.108117

46	6	4.864167	-0.548500	-0.309856
47	8	5.093909	0.601130	-0.647870
48	6	7.178422	-1.137762	-0.752459
49	1	7.134143	-0.766013	-1.776353
50	1	7.552614	-0.351099	-0.097089
51	1	7.828736	-2.008038	-0.699139
52	1	2.900679	-0.147038	0.168548
53	8	0.808120	1.665396	2.228765
54	1	1.125491	0.811423	2.562515

23. Int9’

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.420396	3.149591	-0.406281
2	6	2.408212	2.211223	-0.393867
3	1	3.379001	2.406324	-0.835931
4	7	2.079606	1.076049	0.163093
5	6	0.755246	1.264161	0.716293
6	6	-0.272830	0.217016	0.359173
7	8	-0.014951	-0.986208	0.209089
8	7	-1.545077	0.700366	0.269319
9	1	-2.303710	-0.009742	0.159793
10	6	-1.872796	2.047578	0.212954
11	7	-3.174035	2.358651	0.278640
12	1	-3.892230	1.630392	0.337146
13	1	-3.428228	3.330508	0.132989

14	7	-0.947582	2.987410	0.045104
15	6	0.306807	2.560705	0.145742
16	6	1.433104	4.439494	-1.075879
17	1	0.711688	4.436830	-1.896233
18	1	1.174068	5.225981	-0.365026
19	1	2.433521	4.618667	-1.467033
20	7	-5.914120	-1.756750	-0.169414
21	6	-5.671941	-3.037357	-0.554197
22	1	-6.545766	-3.655161	-0.727266
23	6	-4.408714	-3.504574	-0.708801
24	1	-4.218286	-4.524156	-1.013763
25	6	-3.344330	-2.585025	-0.443236
26	7	-2.069515	-2.969453	-0.562475
27	1	-1.317690	-2.321413	-0.334021
28	1	-1.843627	-3.915292	-0.828418
29	7	-3.584912	-1.323979	-0.071294
30	6	-4.858229	-0.877320	0.070670
31	8	-5.124183	0.287415	0.408902
32	6	-7.275279	-1.248488	-0.003299
33	1	-7.411765	-0.891699	1.018011
34	1	-7.447810	-0.422513	-0.694378
35	1	-7.973005	-2.058009	-0.210162
36	7	6.145410	-1.377806	-0.239169
37	6	5.913166	-2.685779	0.050378

38	1	6.784289	-3.330384	0.036266
39	6	4.675918	-3.167613	0.336063
40	1	4.516667	-4.213359	0.555556
41	6	3.591361	-2.245450	0.325571
42	7	2.341173	-2.591988	0.575860
43	1	1.562017	-1.930713	0.494862
44	1	2.126972	-3.556568	0.785954
45	7	3.860678	-0.952684	0.046046
46	6	5.112610	-0.452871	-0.249025
47	8	5.291693	0.727613	-0.501573
48	6	7.486610	-0.875162	-0.550920
49	1	7.485664	-0.431609	-1.546743
50	1	7.772238	-0.120101	0.181843
51	1	8.181799	-1.711151	-0.515760
52	1	3.093866	-0.196643	0.100109
53	8	0.801861	1.365706	2.152904
54	1	1.242835	0.570945	2.492664
55	8	-2.674130	5.219720	-0.367581
56	1	-1.844669	4.723074	-0.238851
57	1	-2.637789	5.972745	0.232736

24. TS6’

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.431145	3.156733	-0.460891
2	6	2.402171	2.203737	-0.421735

3	1	3.370488	2.362935	-0.882943
4	7	2.064652	1.103650	0.197679
5	6	0.750958	1.331910	0.762498
6	6	-0.285505	0.271820	0.427501
7	8	-0.018021	-0.930298	0.349305
8	7	-1.557736	0.735447	0.274486
9	1	-2.309672	0.013104	0.177532
10	6	-1.922235	2.071104	0.172532
11	7	-3.167285	2.467130	0.163316
12	1	-3.888175	1.748536	0.259877
13	1	-3.153845	3.733518	-0.006308
14	7	-0.949672	3.008966	0.025259
15	6	0.336143	2.632922	0.183405
16	6	1.463117	4.427194	-1.166975
17	1	0.679435	4.442797	-1.928201
18	1	1.309503	5.248001	-0.464283
19	1	2.436058	4.533789	-1.644203
20	7	-5.886855	-1.735492	-0.226961
21	6	-5.632180	-3.009065	-0.625251
22	1	-6.499789	-3.623873	-0.836517
23	6	-4.364513	-3.474496	-0.747290
24	1	-4.164410	-4.488959	-1.062926
25	6	-3.309807	-2.559524	-0.432708
26	7	-2.031109	-2.942683	-0.518071

27	1	-1.288856	-2.299650	-0.252080
28	1	-1.795485	-3.884366	-0.789974
29	7	-3.561509	-1.305330	-0.047582
30	6	-4.839538	-0.858020	0.062762
31	8	-5.114809	0.298892	0.412540
32	6	-7.252638	-1.230360	-0.095309
33	1	-7.422496	-0.893292	0.927733
34	1	-7.403030	-0.390949	-0.775327
35	1	-7.943205	-2.035371	-0.340335
36	7	6.088545	-1.404664	-0.299254
37	6	5.865808	-2.701149	0.044019
38	1	6.732804	-3.350527	0.010422
39	6	4.641865	-3.167084	0.404176
40	1	4.489624	-4.203958	0.666526
41	6	3.561573	-2.240528	0.415590
42	7	2.324634	-2.571252	0.741641
43	1	1.547497	-1.909029	0.668825
44	1	2.116673	-3.525930	0.997900
45	7	3.820578	-0.959885	0.076098
46	6	5.059102	-0.476226	-0.294788
47	8	5.229360	0.693628	-0.597200
48	6	7.416196	-0.917463	-0.685491
49	1	7.377101	-0.520717	-1.700123
50	1	7.727404	-0.129152	0.000193

51	1	8.114018	-1.750538	-0.637066
52	1	3.061839	-0.200896	0.138647
53	8	0.802294	1.430223	2.195055
54	1	1.252366	0.639640	2.532995
55	8	-2.588553	4.794365	-0.227501
56	1	-1.486110	4.064370	-0.104829
57	1	-2.712728	5.429070	0.489204

25. Int10’

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.385085	3.150668	-0.525123
2	6	2.342925	2.188766	-0.486115
3	1	3.288170	2.310446	-1.004788
4	7	2.037209	1.134158	0.215629
5	6	0.744205	1.392148	0.823371
6	6	-0.292782	0.320878	0.490951
7	8	-0.004038	-0.877860	0.469279
8	7	-1.555958	0.759853	0.279735
9	1	-2.286112	0.019600	0.177783
10	6	-1.983172	2.094712	0.188225
11	7	-3.211841	2.452579	0.176611
12	1	-3.853965	1.660062	0.267921
13	1	-3.310886	4.309413	-0.043512
14	7	-0.979254	3.032922	0.063834
15	6	0.337792	2.712333	0.266751

16	6	1.414722	4.399847	-1.267020
17	1	0.573981	4.433003	-1.964364
18	1	1.357865	5.246153	-0.579604
19	1	2.347803	4.448393	-1.826330
20	7	-5.790550	-1.889353	-0.257912
21	6	-5.485488	-3.140289	-0.690633
22	1	-6.327721	-3.781959	-0.923688
23	6	-4.200338	-3.553636	-0.818486
24	1	-3.960282	-4.550783	-1.160606
25	6	-3.183253	-2.608299	-0.471173
26	7	-1.889684	-2.939692	-0.558897
27	1	-1.178902	-2.281852	-0.248555
28	1	-1.615659	-3.866499	-0.845276
29	7	-3.483416	-1.375993	-0.053826
30	6	-4.778297	-0.980041	0.061971
31	8	-5.097235	0.155133	0.441277
32	6	-7.175101	-1.441089	-0.118164
33	1	-7.361549	-1.140181	0.913283
34	1	-7.355593	-0.588861	-0.774573
35	1	-7.833657	-2.264537	-0.389005
36	7	6.049544	-1.386517	-0.331580
37	6	5.845446	-2.673462	0.056237
38	1	6.714741	-3.319165	0.013985
39	6	4.636032	-3.135160	0.467552

40	1	4.498191	-4.164691	0.764425
41	6	3.550945	-2.214616	0.485049
42	7	2.325802	-2.541566	0.855600
43	1	1.546933	-1.881729	0.788456
44	1	2.128978	-3.489182	1.144637
45	7	3.792259	-0.942328	0.102909
46	6	5.015297	-0.463670	-0.323013
47	8	5.168144	0.696759	-0.667433
48	6	7.360746	-0.904895	-0.776810
49	1	7.288646	-0.551844	-1.805776
50	1	7.683623	-0.085714	-0.134209
51	1	8.067939	-1.729057	-0.713560
52	1	3.033339	-0.187665	0.166862
53	8	0.824600	1.465945	2.244116
54	1	1.211801	0.638372	2.570723
55	8	-2.874615	5.171840	-0.229124
56	1	-1.300845	4.000463	-0.029147
57	1	-3.144127	5.778998	0.468985

26. Int11

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.480849	2.713264	-1.104714
2	6	2.358019	1.691155	-0.939646
3	1	3.314898	1.676892	-1.450293
4	7	1.956972	0.746161	-0.132340

5	6	0.694839	1.181430	0.422290
6	6	-0.442292	0.181242	0.231355
7	8	-0.267108	-1.035953	0.330563
8	7	-1.658730	0.719608	-0.013247
9	1	-2.459927	0.051094	-0.009028
10	6	-1.966366	2.084951	-0.197742
11	7	-3.144115	2.568689	-0.152954
12	1	-3.839256	1.848014	0.062288
13	1	-1.053023	3.902194	-0.482554
14	7	-0.882418	2.894406	-0.489240
15	6	0.398324	2.451890	-0.286286
16	6	1.651687	3.895665	-1.932720
17	1	0.731787	4.072113	-2.494323
18	1	1.870771	4.765106	-1.310290
19	1	2.470716	3.716382	-2.627971
20	7	-6.148048	-1.534454	-0.093370
21	6	-5.985244	-2.837844	-0.438851
22	1	-6.895193	-3.407780	-0.588710
23	6	-4.753121	-3.386023	-0.582776
24	1	-4.626477	-4.424741	-0.854592
25	6	-3.634688	-2.523248	-0.351152
26	7	-2.383765	-2.986128	-0.465258
27	1	-1.599999	-2.380319	-0.234811
28	1	-2.212805	-3.953300	-0.692033

29	7	-3.794987	-1.240498	-0.018530
30	6	-5.038775	-0.709855	0.118893
31	8	-5.228696	0.474681	0.424900
32	6	-7.474585	-0.939850	0.061587
33	1	-7.587322	-0.551024	1.074230
34	1	-7.596881	-0.120621	-0.648073
35	1	-8.222140	-1.708669	-0.126320
36	7	5.763318	-2.131897	-0.204066
37	6	5.433828	-3.344587	0.314613
38	1	6.245824	-4.058404	0.390066
39	6	4.173378	-3.657336	0.712767
40	1	3.937396	-4.630591	1.117767
41	6	3.171035	-2.656984	0.572109
42	7	1.908563	-2.839043	0.915144
43	1	1.193048	-2.125582	0.751398
44	1	1.619887	-3.728407	1.297051
45	7	3.536404	-1.461230	0.062263
46	6	4.812329	-1.134404	-0.351945
47	8	5.077371	-0.037803	-0.816346
48	6	7.128199	-1.812998	-0.633563
49	1	7.129264	-1.577081	-1.697954
50	1	7.494229	-0.953833	-0.071370
51	1	7.757865	-2.679220	-0.442409
52	1	2.843019	-0.646552	0.003835

53	8	0.791994	1.435595	1.835409
54	1	1.212686	0.670663	2.259865
55	8	1.686395	4.178288	1.932483
56	1	1.426161	3.248292	2.056515
57	1	1.898213	4.519619	2.809445
58	8	-0.211747	5.479693	0.350822
59	1	0.480516	5.129648	0.947477
60	1	0.083383	6.348747	0.058741

27. TS7

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.564297	2.873720	-0.899951
2	6	2.518078	1.898068	-0.716012
3	1	3.557431	2.060468	-0.970432
4	7	2.024466	0.776218	-0.249784
5	6	0.690800	1.043346	0.018445
6	6	-0.398863	0.055558	0.002048
7	8	-0.228892	-1.161870	0.110963
8	7	-1.634665	0.612683	-0.134842
9	1	-2.440191	-0.046913	-0.070740
10	6	-1.942690	1.976852	-0.279164
11	7	-3.107312	2.479082	-0.211737
12	1	-3.813766	1.767543	0.002746
13	1	-1.041985	3.826943	-0.590506
14	7	-0.857465	2.814088	-0.567368

15	6	0.388809	2.324363	-0.520990
16	6	1.790254	4.237859	-1.363915
17	1	0.974424	4.528426	-2.027111
18	1	1.836023	4.907963	-0.504038
19	1	2.729531	4.261063	-1.914052
20	7	-6.147839	-1.595261	-0.032166
21	6	-6.008511	-2.914868	-0.322495
22	1	-6.928318	-3.479328	-0.425785
23	6	-4.786682	-3.484097	-0.470614
24	1	-4.678728	-4.535128	-0.699806
25	6	-3.652804	-2.625948	-0.304961
26	7	-2.411220	-3.109534	-0.429314
27	1	-1.613000	-2.500665	-0.264870
28	1	-2.257863	-4.086336	-0.625292
29	7	-3.790355	-1.327846	-0.024375
30	6	-5.024412	-0.776897	0.117702
31	8	-5.194099	0.422638	0.375575
32	6	-7.463388	-0.977478	0.126220
33	1	-7.550598	-0.548102	1.124906
34	1	-7.589951	-0.185150	-0.612586
35	1	-8.224148	-1.743075	-0.016358
36	7	5.940842	-1.993173	-0.091110
37	6	5.607661	-3.246565	0.318355
38	1	6.433147	-3.941803	0.417523

39	6	4.329409	-3.619854	0.587203
40	1	4.092854	-4.624108	0.907671
41	6	3.308704	-2.641080	0.427030
42	7	2.029745	-2.876768	0.653708
43	1	1.302160	-2.174634	0.488582
44	1	1.741513	-3.795506	0.959299
45	7	3.679315	-1.407319	0.020585
46	6	4.974736	-1.013968	-0.254099
47	8	5.237689	0.121133	-0.614083
48	6	7.326519	-1.606105	-0.374297
49	1	7.406661	-1.276992	-1.410421
50	1	7.618909	-0.791833	0.288976
51	1	7.964673	-2.470943	-0.206979
52	1	2.972480	-0.624581	-0.074491
53	8	0.563698	1.433988	1.825526
54	1	1.321514	0.932383	2.165409
55	8	0.971833	4.117272	1.836565
56	1	0.831807	3.141672	1.931703
57	1	1.189636	4.450504	2.714461
58	8	-0.857203	5.444629	0.262798
59	1	-0.204070	5.134883	0.925387
60	1	-0.548735	6.294587	-0.070185

28. Int12

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	1.579244	2.920144	-0.822255
2	6	2.545698	1.949909	-0.646649
3	1	3.596056	2.154659	-0.807562
4	7	2.048435	0.789633	-0.297387
5	6	0.699999	1.003267	-0.161535
6	6	-0.377299	0.031265	-0.076618
7	8	-0.210646	-1.181671	0.088034
8	7	-1.618119	0.586453	-0.207308
9	1	-2.420560	-0.071105	-0.109626
10	6	-1.931609	1.947001	-0.353772
11	7	-3.097902	2.444530	-0.305309
12	1	-3.806453	1.730783	-0.104333
13	1	-1.041514	3.815882	-0.605881
14	7	-0.845801	2.801558	-0.613320
15	6	0.398015	2.322758	-0.557356
16	6	1.804030	4.315769	-1.188109
17	1	1.019711	4.631939	-1.876942
18	1	1.791580	4.930059	-0.286999
19	1	2.769981	4.384988	-1.685721
20	7	-6.133454	-1.636724	-0.021781
21	6	-5.988134	-2.968981	-0.243288
22	1	-6.905428	-3.541550	-0.321432
23	6	-4.763584	-3.540028	-0.357254
24	1	-4.650657	-4.600868	-0.532461

25	6	-3.633608	-2.669949	-0.231184
26	7	-2.389972	-3.155011	-0.324935
27	1	-1.594485	-2.534563	-0.193470
28	1	-2.232489	-4.139700	-0.472076
29	7	-3.776768	-1.359587	-0.018321
30	6	-5.013601	-0.807341	0.089648
31	8	-5.189572	0.403330	0.284080
32	6	-7.451980	-1.017082	0.100522
33	1	-7.543587	-0.536009	1.074942
34	1	-7.580241	-0.265455	-0.679397
35	1	-8.209022	-1.792600	-0.002939
36	7	5.984734	-1.971536	-0.066354
37	6	5.648845	-3.237010	0.301872
38	1	6.475911	-3.930236	0.402206
39	6	4.366970	-3.623757	0.531570
40	1	4.128857	-4.637451	0.819660
41	6	3.343893	-2.647250	0.372790
42	7	2.061713	-2.896322	0.561757
43	1	1.332216	-2.192523	0.411042
44	1	1.773219	-3.824821	0.836393
45	7	3.718232	-1.401378	0.007164
46	6	5.018013	-0.992547	-0.224141
47	8	5.281645	0.153871	-0.544406
48	6	7.374600	-1.571697	-0.308702

49	1	7.471831	-1.200477	-1.328885
50	1	7.654758	-0.785345	0.392462
51	1	8.010477	-2.442601	-0.166666
52	1	3.011933	-0.626616	-0.099952
53	8	0.395172	1.563144	1.870173
54	1	1.170821	1.087294	2.207424
55	8	0.772576	4.190132	1.864008
56	1	0.642029	3.202109	1.932156
57	1	0.918913	4.512071	2.760547
58	8	-1.006526	5.424892	0.206358
59	1	-0.374026	5.155129	0.908041
60	1	-0.704909	6.269145	-0.146921

29. Int13

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.620492	2.958104	-0.707332
2	6	2.577979	1.977810	-0.539333
3	1	3.635106	2.190730	-0.630145
4	7	2.065138	0.799498	-0.286057
5	6	0.711213	1.006335	-0.210280
6	6	-0.368866	0.034295	-0.223099
7	8	-0.208763	-1.185118	-0.111085
8	7	-1.603573	0.598706	-0.379029
9	1	-2.409498	-0.055164	-0.310151
10	6	-1.909267	1.966906	-0.467063

11	7	-3.075449	2.465752	-0.450680
12	1	-3.797000	1.744054	-0.346634
13	1	-1.009900	3.843530	-0.579500
14	7	-0.811747	2.830973	-0.626835
15	6	0.428107	2.347769	-0.539076
16	6	1.861475	4.373035	-0.976540
17	1	1.119599	4.728839	-1.692683
18	1	1.792090	4.932986	-0.043150
19	1	2.855705	4.471517	-1.408994
20	7	-6.146791	-1.628902	-0.012682
21	6	-5.996400	-2.967502	0.161740
22	1	-6.911424	-3.541521	0.254816
23	6	-4.769431	-3.541494	0.215751
24	1	-4.651179	-4.606941	0.356176
25	6	-3.643221	-2.667469	0.080186
26	7	-2.398736	-3.156828	0.122947
27	1	-1.604930	-2.526671	0.034929
28	1	-2.238636	-4.143165	0.255052
29	7	-3.790399	-1.351446	-0.092200
30	6	-5.030083	-0.797393	-0.141561
31	8	-5.213953	0.417826	-0.296949
32	6	-7.467921	-1.005750	-0.071043
33	1	-7.567644	-0.275739	0.733149
34	1	-7.593992	-0.498149	-1.028030

35	1	-8.221535	-1.783808	0.038188
36	7	6.004856	-1.950855	-0.015199
37	6	5.657116	-3.258846	0.117870
38	1	6.482262	-3.958380	0.184035
39	6	4.365970	-3.678486	0.164889
40	1	4.118606	-4.725144	0.267827
41	6	3.346436	-2.690119	0.071873
42	7	2.056747	-2.967291	0.109092
43	1	1.333020	-2.246025	0.033697
44	1	1.759729	-3.927500	0.210379
45	7	3.732163	-1.402014	-0.061179
46	6	5.040946	-0.961631	-0.117122
47	8	5.314708	0.219393	-0.246052
48	6	7.404407	-1.515619	-0.058670
49	1	7.599564	-1.012580	-1.005903
50	1	7.595648	-0.827120	0.764612
51	1	8.038652	-2.394314	0.035161
52	1	3.025990	-0.622631	-0.129936
53	8	0.304917	1.460605	1.837467
54	1	1.068827	0.972506	2.183887
55	8	0.658072	4.087432	1.992348
56	1	0.532352	3.096593	2.000558
57	1	0.760093	4.360954	2.910778
58	8	-1.028538	5.414828	0.306241

59	1	-0.436899	5.109082	1.028145
60	1	-0.705812	6.273409	0.010900

30. TS8

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.601626	2.998697	-0.639903
2	6	2.558560	2.034570	-0.496082
3	1	3.616387	2.263790	-0.509270
4	7	2.056797	0.813413	-0.358578
5	6	0.725846	0.980988	-0.387567
6	6	-0.347502	0.001504	-0.292609
7	8	-0.161051	-1.205295	-0.124800
8	7	-1.585674	0.550885	-0.438143
9	1	-2.386907	-0.111060	-0.339711
10	6	-1.902828	1.915146	-0.532391
11	7	-3.075380	2.398438	-0.528331
12	1	-3.791204	1.666611	-0.432816
13	1	-1.045641	3.850949	-0.524307
14	7	-0.823804	2.811524	-0.672063
15	6	0.408277	2.351307	-0.583093
16	6	1.828017	4.436852	-0.785077
17	1	1.171888	4.819684	-1.567120
18	1	1.622951	4.921338	0.170369
19	1	2.865337	4.584479	-1.079936
20	7	-6.091518	-1.686209	-0.019730

21	6	-5.935729	-3.014192	0.219637
22	1	-6.848393	-3.588447	0.331740
23	6	-4.706258	-3.577752	0.311532
24	1	-4.583535	-4.634672	0.503068
25	6	-3.583274	-2.705627	0.144074
26	7	-2.337650	-3.187089	0.218998
27	1	-1.545334	-2.560778	0.102926
28	1	-2.174968	-4.165786	0.397085
29	7	-3.736059	-1.399341	-0.090716
30	6	-4.978631	-0.856368	-0.176667
31	8	-5.167323	0.349799	-0.389990
32	6	-7.415263	-1.072993	-0.118318
33	1	-7.527216	-0.310739	0.653712
34	1	-7.532694	-0.606498	-1.096993
35	1	-8.166173	-1.849872	0.014892
36	7	6.054838	-1.872042	0.004426
37	6	5.739629	-3.188792	0.133494
38	1	6.582218	-3.866087	0.209451
39	6	4.459643	-3.643366	0.165987
40	1	4.239141	-4.696085	0.267747
41	6	3.415261	-2.683323	0.060759
42	7	2.132689	-2.992067	0.083854
43	1	1.395238	-2.287081	0.007157
44	1	1.856397	-3.958610	0.183341

45	7	3.770204	-1.385850	-0.070007
46	6	5.067370	-0.908405	-0.108186
47	8	5.307960	0.280047	-0.231348
48	6	7.443255	-1.400182	-0.023031
49	1	7.634074	-0.888207	-0.966300
50	1	7.608102	-0.710660	0.805046
51	1	8.099307	-2.262438	0.073262
52	1	3.050686	-0.631925	-0.158827
53	8	0.110101	1.728278	1.892074
54	1	0.801070	1.302263	2.414637
55	8	0.303660	4.137594	1.985697
56	1	0.225205	2.981282	1.988647
57	1	0.224924	4.449654	2.893951
58	8	-1.189024	5.207141	0.254570
59	1	-0.595691	4.898543	1.035299
60	1	-0.850477	6.041107	-0.090086

31. Int14

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.609223	2.995589	-0.676202
2	6	2.576900	2.070430	-0.516065
3	1	3.631129	2.315462	-0.506373
4	7	2.098309	0.829856	-0.381320
5	6	0.763420	0.963304	-0.460943
6	6	-0.290939	-0.025014	-0.361318

7	8	-0.107262	-1.236602	-0.178005
8	7	-1.527910	0.521988	-0.515718
9	1	-2.326255	-0.136876	-0.418063
10	6	-1.824720	1.895493	-0.630502
11	7	-3.033525	2.339699	-0.669135
12	1	-3.722369	1.578394	-0.602518
13	1	-1.432924	4.611616	-0.224400
14	7	-0.799782	2.820555	-0.723352
15	6	0.407530	2.315668	-0.637421
16	6	1.765919	4.437211	-0.834104
17	1	1.147868	4.768531	-1.669057
18	1	1.457704	4.931643	0.087796
19	1	2.812765	4.648366	-1.045370
20	7	-6.038272	-1.758347	-0.058740
21	6	-5.867157	-3.064276	0.273867
22	1	-6.773271	-3.640956	0.421059
23	6	-4.631289	-3.604422	0.411180
24	1	-4.496622	-4.643882	0.676273
25	6	-3.518298	-2.731344	0.188345
26	7	-2.266235	-3.188324	0.302073
27	1	-1.481952	-2.560050	0.138987
28	1	-2.091451	-4.150966	0.544561
29	7	-3.686360	-1.447064	-0.137093
30	6	-4.934222	-0.926828	-0.267381

31	8	-5.135672	0.259193	-0.565153
32	6	-7.368814	-1.170859	-0.206512
33	1	-7.494074	-0.356480	0.508147
34	1	-7.487348	-0.777182	-1.216620
35	1	-8.110925	-1.945444	-0.020611
36	7	6.122136	-1.791643	0.028985
37	6	5.812115	-3.109818	0.157274
38	1	6.656941	-3.782735	0.246209
39	6	4.534131	-3.569664	0.174091
40	1	4.317046	-4.623011	0.276609
41	6	3.486323	-2.614201	0.052075
42	7	2.205881	-2.932080	0.058129
43	1	1.458961	-2.234849	-0.030576
44	1	1.938620	-3.901502	0.154438
45	7	3.835400	-1.315134	-0.077161
46	6	5.130601	-0.833191	-0.097687
47	8	5.369539	0.356215	-0.218764
48	6	7.508144	-1.312971	0.016936
49	1	7.707624	-0.801623	-0.924920
50	1	7.660274	-0.620941	0.845397
51	1	8.167609	-2.171607	0.122403
52	1	3.108520	-0.560258	-0.177701
53	8	-0.488442	1.479929	2.207017
54	1	-1.332668	1.411152	2.666092

55	8	0.283428	4.150217	2.084810
56	1	-0.249882	2.428107	2.229017
57	1	0.458510	4.584513	2.927546
58	8	-1.521357	5.357128	0.399945
59	1	-0.374549	4.704323	1.614353
60	1	-1.281059	6.154843	-0.085752

32. Int15

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.551083	3.282386	0.000348
2	6	-2.573544	2.369471	0.000838
3	1	-3.614221	2.664670	0.001454
4	7	-2.141957	1.131252	0.000557
5	6	-0.768208	1.232829	-0.000196
6	6	0.245499	0.236842	-0.000818
7	8	0.086458	-0.996952	-0.001037
8	7	1.522034	0.781338	-0.001231
9	1	2.308360	0.096768	-0.001338
10	6	1.807644	2.126746	-0.001200
11	7	3.097593	2.471872	-0.001664
12	1	3.848198	1.770663	-0.001687
13	1	3.322623	3.457739	-0.001616
14	7	0.863808	3.064382	-0.000796
15	6	-0.389114	2.566195	-0.000287
16	6	-1.655007	4.734962	0.000401

17	1	-1.173875	5.138219	0.892836
18	1	-1.175092	5.138198	-0.892700
19	1	-2.709751	5.004875	0.001119
20	7	6.023785	-1.545189	0.001417
21	6	5.837385	-2.891237	0.002518
22	1	6.736944	-3.495910	0.003659
23	6	4.595651	-3.434238	0.002208
24	1	4.449233	-4.505376	0.003131
25	6	3.492165	-2.521918	0.000684
26	7	2.236207	-2.977675	0.000310
27	1	1.455499	-2.321903	-0.000483
28	1	2.052491	-3.968964	0.001166
29	7	3.677322	-1.197371	-0.000444
30	6	4.930645	-0.679201	-0.000099
31	8	5.149858	0.543840	-0.001090
32	6	7.362347	-0.956205	0.001799
33	1	7.493059	-0.337533	-0.886665
34	1	7.491813	-0.335869	0.889286
35	1	8.093087	-1.763228	0.003074
36	7	-6.184937	-1.446706	0.001155
37	6	-5.880393	-2.772415	-0.001820
38	1	-6.727896	-3.448046	-0.002562
39	6	-4.603390	-3.234046	-0.003713
40	1	-4.387729	-4.292805	-0.006071

41	6	-3.552469	-2.272727	-0.002529
42	7	-2.273592	-2.599520	-0.004419
43	1	-1.513690	-1.907822	-0.003054
44	1	-2.017529	-3.576659	-0.006795
45	7	-3.893987	-0.965892	0.000714
46	6	-5.188160	-0.483720	0.002255
47	8	-5.428050	0.712216	0.004560
48	6	-7.569023	-0.963435	0.002810
49	1	-7.742076	-0.359226	0.893570
50	1	-7.743454	-0.356948	-0.886144
51	1	-8.232809	-1.825153	0.002223
52	1	-3.154916	-0.196617	0.000904
53	8	2.098955	5.534955	-0.001328
54	1	1.505443	4.728898	-0.000896

33. Int16

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.549424	3.330919	0.003478
2	6	-2.546703	2.423890	0.001767
3	1	-3.593773	2.698259	0.003601
4	7	-2.106736	1.162181	-0.002373
5	6	-0.766356	1.262574	-0.003246
6	6	0.257187	0.236906	-0.006924
7	8	0.038869	-0.980943	-0.010078
8	7	1.515016	0.767432	-0.006395

9	1	2.296509	0.077336	-0.007286
10	6	1.846266	2.138595	-0.002989
11	7	3.070171	2.544303	-0.003116
12	1	3.750599	1.771632	-0.006330
13	1	3.115759	4.468605	0.002047
14	7	0.851382	3.099643	0.000716
15	6	-0.366894	2.615521	0.000378
16	6	-1.655335	4.785762	0.007963
17	1	-1.171569	5.178688	0.902490
18	1	-1.170322	5.184162	-0.883452
19	1	-2.710238	5.053004	0.008023
20	7	5.957835	-1.658736	0.002226
21	6	5.753865	-3.001674	0.010969
22	1	6.645280	-3.618412	0.016194
23	6	4.504937	-3.528621	0.012995
24	1	4.344042	-4.597679	0.020167
25	6	3.414289	-2.601050	0.005346
26	7	2.151788	-3.042175	0.006975
27	1	1.382381	-2.376273	0.000684
28	1	1.953763	-4.030505	0.012793
29	7	3.614810	-1.280233	-0.003537
30	6	4.875668	-0.775266	-0.005259
31	8	5.107710	0.442558	-0.013374
32	6	7.303625	-1.087358	0.000092

33	1	7.443607	-0.476643	-0.892547
34	1	7.440006	-0.461880	0.882990
35	1	8.024406	-1.903336	0.008355
36	7	-6.211500	-1.358405	0.002134
37	6	-5.951563	-2.693364	0.000500
38	1	-6.821871	-3.338995	0.001802
39	6	-4.691588	-3.200913	-0.002629
40	1	-4.515060	-4.266595	-0.003919
41	6	-3.607656	-2.279131	-0.004294
42	7	-2.339543	-2.644337	-0.007697
43	1	-1.568776	-1.969705	-0.008501
44	1	-2.107671	-3.627719	-0.009570
45	7	-3.907457	-0.961342	-0.002219
46	6	-5.183945	-0.430385	0.001067
47	8	-5.376522	0.773350	0.002750
48	6	-7.579522	-0.829927	0.005155
49	1	-7.731949	-0.221785	0.896919
50	1	-7.734032	-0.217512	-0.883306
51	1	-8.270398	-1.670161	0.003913
52	1	-3.155415	-0.227836	-0.002886
53	8	2.888581	5.420087	0.005136
54	1	1.923577	5.404830	0.005657

34. Int15’

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z

1	7	-1.469168	3.164596	-0.059013
2	6	-2.552231	2.324835	-0.044717
3	1	-3.569979	2.691063	-0.060101
4	7	-2.207707	1.060449	-0.014320
5	6	-0.830774	1.067425	-0.006786
6	6	0.107533	0.001626	0.014116
7	8	-0.141471	-1.217598	0.038099
8	7	1.417668	0.453486	0.001343
9	1	2.151301	-0.285342	0.004125
10	6	1.803565	1.776380	-0.026514
11	7	3.116945	2.010439	-0.037929
12	1	3.795523	1.240221	-0.043338
13	1	3.457385	2.963571	-0.118876
14	7	0.929141	2.780360	-0.038057
15	6	-0.357114	2.370455	-0.033204
16	6	-1.486501	4.620693	-0.083573
17	1	-1.167452	5.016509	0.882137
18	1	-0.817703	4.977661	-0.867645
19	1	-2.503137	4.949057	-0.294353
20	7	5.735624	-2.227270	-0.014439
21	6	5.442381	-3.554255	0.011296
22	1	6.290394	-4.229561	0.011379
23	6	4.161231	-3.995772	0.035314
24	1	3.928673	-5.051628	0.055932

25	6	3.134450	-2.997495	0.032333
26	7	1.846233	-3.351056	0.055635
27	1	1.120425	-2.634823	0.051605
28	1	1.584120	-4.324130	0.073704
29	7	3.424187	-1.692332	0.006702
30	6	4.714825	-1.276233	-0.017184
31	8	5.029947	-0.074850	-0.041457
32	6	7.116149	-1.745081	-0.039547
33	1	7.283294	-1.152929	-0.939953
34	1	7.304503	-1.121979	0.835439
35	1	7.782670	-2.605762	-0.032441
36	7	-6.417449	-1.215051	-0.013322
37	6	-6.214170	-2.559409	0.002826
38	1	-7.110683	-3.168134	0.001282
39	6	-4.976207	-3.116888	0.019818
40	1	-4.843723	-4.188772	0.032462
41	6	-3.855131	-2.238622	0.020284
42	7	-2.604692	-2.661594	0.035879
43	1	-1.795840	-2.027496	0.035876
44	1	-2.422924	-3.655567	0.048178
45	7	-4.096678	-0.909747	0.004235
46	6	-5.350507	-0.330745	-0.014170
47	8	-5.499061	0.879873	-0.030013
48	6	-7.762012	-0.631771	-0.032545

49	1	-7.897777	-0.001312	0.846351
50	1	-7.885231	-0.029993	-0.933203
51	1	-8.486104	-1.443694	-0.024536
52	1	-3.302614	-0.196325	0.000241
53	8	4.339521	4.823863	-0.243075
54	1	3.437426	5.202152	-0.022749
55	8	1.810855	5.421184	0.334078
56	1	1.430388	4.514279	0.253322
57	1	1.627072	5.726353	1.230619

35. Int16’

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.466160	3.197269	0.005701
2	6	-2.516688	2.351652	-0.008506
3	1	-3.544930	2.689288	-0.017834
4	7	-2.154261	1.065655	-0.012186
5	6	-0.811918	1.084502	-0.000809
6	6	0.144627	-0.004544	0.005131
7	8	-0.151939	-1.204646	0.001399
8	7	1.433304	0.445017	0.015147
9	1	2.168853	-0.294761	0.015009
10	6	1.855457	1.790444	0.016343
11	7	3.102932	2.109381	0.012079
12	1	3.721098	1.285096	0.010291
13	1	3.955003	3.807936	-0.425642

14	7	0.919558	2.811914	0.021437
15	6	-0.330202	2.411298	0.010840
16	6	-1.493462	4.656520	0.021978
17	1	-1.094011	5.017545	0.970258
18	1	-0.889855	5.034855	-0.803147
19	1	-2.526087	4.980598	-0.093164
20	7	5.706632	-2.267219	0.021090
21	6	5.414879	-3.594184	0.034945
22	1	6.263491	-4.268812	0.040820
23	6	4.133885	-4.037518	0.040711
24	1	3.902110	-5.093670	0.051383
25	6	3.106650	-3.040041	0.031270
26	7	1.818210	-3.397545	0.035875
27	1	1.093680	-2.683443	0.025070
28	1	1.556170	-4.370648	0.044319
29	7	3.393379	-1.735125	0.017860
30	6	4.684819	-1.314729	0.012297
31	8	4.996061	-0.114615	-0.000153
32	6	7.086444	-1.783086	0.014931
33	1	7.262343	-1.183182	-0.878691
34	1	7.264533	-1.166617	0.896789
35	1	7.754399	-2.642688	0.022172
36	7	-6.405376	-1.198380	-0.026833
37	6	-6.232971	-2.547114	-0.023211

38	1	-7.143829	-3.134146	-0.025133
39	6	-5.008983	-3.136414	-0.017499
40	1	-4.904280	-4.211333	-0.014608
41	6	-3.867022	-2.287689	-0.015389
42	7	-2.625080	-2.733934	-0.009798
43	1	-1.813696	-2.109085	-0.007233
44	1	-2.456219	-3.730330	-0.006969
45	7	-4.080796	-0.953187	-0.019228
46	6	-5.319772	-0.339471	-0.024638
47	8	-5.432885	0.874220	-0.027251
48	6	-7.736495	-0.583394	-0.033342
49	1	-7.854855	0.036432	0.855535
50	1	-7.847051	0.034106	-0.924837
51	1	-8.478786	-1.378588	-0.035605
52	1	-3.284232	-0.270959	-0.017835
53	8	4.285218	4.703229	-0.630326
54	1	3.567320	5.273713	-0.311068
55	8	1.792595	5.586325	0.419829
56	1	1.497775	4.659075	0.343943
57	1	1.766778	5.799200	0.005701

36. Int17

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.538124	3.361583	-0.452768
2	6	2.508379	2.398660	-0.494032

3	1	3.556714	2.646930	-0.593350
4	7	2.018246	1.181679	-0.410578
5	6	0.656168	1.357457	-0.307712
6	6	-0.404620	0.418600	-0.215978
7	8	-0.312088	-0.824953	-0.211485
8	7	-1.643249	1.031972	-0.131707
9	1	-2.463400	0.394639	-0.061978
10	6	-1.852147	2.395348	-0.150216
11	7	-3.124089	2.801744	-0.061337
12	1	-3.905682	2.145069	0.039014
13	1	-3.295222	3.795522	-0.065475
14	7	-0.872917	3.282435	-0.254675
15	6	0.341235	2.710681	-0.330913
16	6	1.719701	4.804784	-0.510476
17	1	1.176389	5.208874	-1.365426
18	1	1.347985	5.258544	0.409081
19	1	2.782616	5.014142	-0.618867
20	7	-6.260800	-1.050870	0.258208
21	6	-6.147472	-2.404476	0.214548
22	1	-7.074593	-2.961978	0.284054
23	6	-4.941394	-3.010546	0.091883
24	1	-4.852599	-4.087606	0.058540
25	6	-3.795012	-2.156008	0.012380
26	7	-2.569675	-2.675737	-0.105849

27	1	-1.756253	-2.062006	-0.150091
28	1	-2.440100	-3.674949	-0.136651
29	7	-3.908339	-0.824345	0.052580
30	6	-5.127328	-0.242024	0.172921
31	8	-5.280001	0.990240	0.211276
32	6	-7.559945	-0.392840	0.391316
33	1	-7.566205	0.230074	1.286248
34	1	-7.747274	0.235409	-0.480354
35	1	-8.328307	-1.160180	0.468065
36	7	5.787915	-1.698117	0.179879
37	6	5.442654	-2.963390	-0.187969
38	1	6.252911	-3.682570	-0.208464
39	6	4.170067	-3.314935	-0.501652
40	1	3.921429	-4.328510	-0.781103
41	6	3.168933	-2.303603	-0.442445
42	7	1.896954	-2.521238	-0.710409
43	1	1.167136	-1.808174	-0.570655
44	1	1.603761	-3.451458	-0.975154
45	7	3.556323	-1.054580	-0.092343
46	6	4.842750	-0.696613	0.237313
47	8	5.126872	0.452512	0.562851
48	6	7.166044	-1.334328	0.528334
49	1	7.519255	-0.559091	-0.151509
50	1	7.194269	-0.961570	1.552196

51	1	7.786983	-2.222574	0.436776
52	1	2.889002	-0.223519	-0.180364
53	8	3.242148	1.930786	2.090429
54	1	3.958210	1.424017	1.640088

37. TS9

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.557006	3.352587	-0.459730
2	6	2.527262	2.381421	-0.556382
3	1	3.547483	2.621871	-0.818884
4	7	2.003375	1.157361	-0.588251
5	6	0.667035	1.345052	-0.427375
6	6	-0.404872	0.407002	-0.348577
7	8	-0.318610	-0.830951	-0.425065
8	7	-1.630607	1.022819	-0.173908
9	1	-2.454745	0.388043	-0.106171
10	6	-1.821792	2.386672	-0.081718
11	7	-3.079117	2.796858	0.093209
12	1	-3.869261	2.142778	0.151899
13	1	-3.238008	3.790964	0.159150
14	7	-0.836551	3.274787	-0.157941
15	6	0.365870	2.711248	-0.335138
16	6	1.787481	4.778840	-0.298676
17	1	0.931150	5.317791	-0.702439
18	1	1.911940	5.016596	0.759922

19	1	2.687078	5.054520	-0.847506
20	7	-6.237358	-1.031187	0.317005
21	6	-6.137308	-2.385386	0.259757
22	1	-7.065235	-2.936024	0.364082
23	6	-4.942554	-3.000336	0.082747
24	1	-4.864408	-4.077800	0.038724
25	6	-3.793530	-2.154862	-0.040419
26	7	-2.579464	-2.683937	-0.217873
27	1	-1.765161	-2.076915	-0.301517
28	1	-2.460110	-3.683663	-0.267853
29	7	-3.893570	-0.822546	0.016606
30	6	-5.101345	-0.231779	0.194387
31	8	-5.241103	1.001541	0.253038
32	6	-7.524361	-0.363156	0.508023
33	1	-7.494839	0.239469	1.416382
34	1	-7.732531	0.286279	-0.342992
35	1	-8.298145	-1.124210	0.592307
36	7	5.734959	-1.759175	0.343066
37	6	5.386311	-3.041964	0.050627
38	1	6.178221	-3.775626	0.145424
39	6	4.131157	-3.395197	-0.327164
40	1	3.879909	-4.423452	-0.543615
41	6	3.152404	-2.365332	-0.418564
42	7	1.896756	-2.579965	-0.758806

43	1	1.176348	-1.848262	-0.711197
44	1	1.597643	-3.522241	-0.968124
45	7	3.543552	-1.100288	-0.138174
46	6	4.813090	-0.734907	0.256098
47	8	5.098710	0.427653	0.510506
48	6	7.093830	-1.394453	0.758691
49	1	7.504155	-0.668265	0.057080
50	1	7.063452	-0.958867	1.757536
51	1	7.703247	-2.295331	0.761961
52	1	2.893675	-0.279969	-0.302082
53	8	3.180964	2.407568	1.505041
54	1	3.863515	1.717449	1.375441

38. Int18

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	1.534770	3.319853	-0.214115
2	6	2.619431	2.344381	-0.278280
3	1	3.183485	2.468459	-1.215072
4	7	1.968566	1.039103	-0.254492
5	6	0.660385	1.274538	-0.166068
6	6	-0.431571	0.362780	-0.102783
7	8	-0.354322	-0.883222	-0.116243
8	7	-1.669821	0.988530	-0.026672
9	1	-2.502460	0.361135	0.005209
10	6	-1.846667	2.345401	-0.005847

11	7	-3.096839	2.791729	0.070327
12	1	-3.904779	2.156513	0.119607
13	1	-3.233419	3.791607	0.085352
14	7	-0.840150	3.228664	-0.057584
15	6	0.365835	2.678479	-0.138204
16	6	1.756056	4.750555	-0.219087
17	1	0.785429	5.245918	-0.218146
18	1	2.321574	5.046150	0.667280
19	1	2.311160	5.037341	-1.116089
20	7	-6.320241	-0.978169	0.108448
21	6	-6.239787	-2.331768	0.014556
22	1	-7.183259	-2.865548	0.016302
23	6	-5.045438	-2.966263	-0.075529
24	1	-4.984249	-4.043038	-0.151133
25	6	-3.874489	-2.142192	-0.065220
26	7	-2.658085	-2.688786	-0.146051
27	1	-1.828811	-2.095170	-0.135002
28	1	-2.550754	-3.688969	-0.212657
29	7	-3.956517	-0.810357	0.024830
30	6	-5.163814	-0.199525	0.110664
31	8	-5.285354	1.034752	0.192953
32	6	-7.606929	-0.289892	0.207183
33	1	-7.647071	0.283761	1.133708
34	1	-7.727612	0.389482	-0.637349

35	1	-8.398504	-1.037101	0.198992
36	7	5.833033	-1.730578	0.097600
37	6	5.452789	-3.037345	0.057554
38	1	6.257972	-3.761426	0.098877
39	6	4.153572	-3.419503	-0.027272
40	1	3.876842	-4.463477	-0.057036
41	6	3.164579	-2.395277	-0.077840
42	7	1.871110	-2.641137	-0.159309
43	1	1.157018	-1.900451	-0.164915
44	1	1.554008	-3.600151	-0.184496
45	7	3.581260	-1.109461	-0.039996
46	6	4.896004	-0.717834	0.050960
47	8	5.221129	0.465155	0.086644
48	6	7.241184	-1.330753	0.190840
49	1	7.500819	-0.715583	-0.670644
50	1	7.397101	-0.759202	1.105887
51	1	7.851338	-2.231045	0.203999
52	1	2.875791	-0.289555	-0.120503
53	8	3.460827	2.547404	0.819853
54	1	4.213694	1.937213	0.707521

39. Int19

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.337632	3.252445	-0.163330
2	6	-2.408029	2.261923	-0.100105

3	1	-3.006993	2.416992	0.811541
4	7	-1.737726	0.968768	-0.047743
5	6	-0.430956	1.223221	-0.073041
6	6	0.676440	0.327035	-0.054445
7	8	0.616985	-0.918598	-0.008838
8	7	1.906916	0.970821	-0.087262
9	1	2.749704	0.356757	-0.059945
10	6	2.064351	2.329595	-0.143836
11	7	3.309855	2.793541	-0.166401
12	1	4.128944	2.170484	-0.151662
13	1	3.432173	3.794400	-0.211368
14	7	1.043625	3.197146	-0.178308
15	6	-0.156529	2.629848	-0.142650
16	6	-1.582548	4.678619	-0.211540
17	1	-0.620427	5.190155	-0.216478
18	1	-2.139185	4.931376	-1.116296
19	1	-2.156099	4.988289	0.666271
20	7	6.589173	-0.921492	0.012294
21	6	6.526355	-2.275712	0.110386
22	1	7.477481	-2.794573	0.145351
23	6	5.339435	-2.928300	0.160648
24	1	5.291985	-4.005615	0.238334
25	6	4.157064	-2.122613	0.104104
26	7	2.947111	-2.687728	0.144806

27	1	2.109799	-2.107771	0.095094
28	1	2.852790	-3.689084	0.213753
29	7	4.221696	-0.790123	0.009581
30	6	5.421781	-0.161114	-0.036845
31	8	5.527449	1.074421	-0.122853
32	6	7.867895	-0.213949	-0.044984
33	1	7.934676	0.350939	-0.975406
34	1	7.945469	0.475744	0.796193
35	1	8.670001	-0.948390	0.001521
36	7	-5.535193	-1.862542	-0.405595
37	6	-5.140835	-3.165633	-0.382097
38	1	-5.938040	-3.897740	-0.435093
39	6	-3.837815	-3.535233	-0.296751
40	1	-3.550926	-4.576603	-0.275102
41	6	-2.859953	-2.501504	-0.225586
42	7	-1.564932	-2.733122	-0.126103
43	1	-0.863715	-1.982057	-0.080331
44	1	-1.235966	-3.688201	-0.104009
45	7	-3.289919	-1.220773	-0.262490
46	6	-4.608417	-0.841524	-0.344676
47	8	-4.942627	0.339652	-0.358290
48	6	-6.947466	-1.475730	-0.491724
49	1	-7.213675	-0.880359	0.381649
50	1	-7.108603	-0.887787	-1.395376

51	1	-7.548333	-2.381801	-0.523258
52	1	-2.599589	-0.388545	-0.175459
53	8	-3.217272	2.406827	-1.230358
54	1	-3.974584	1.806365	-1.102130
55	8	-4.039928	1.114547	2.560734
56	8	-3.318650	0.183758	2.335219

40. TS10

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.367317	3.224852	-0.332290
2	6	-2.379865	2.204915	-0.290713
3	1	-2.743831	2.124586	0.887310
4	7	-1.737057	0.967163	-0.447319
5	6	-0.446499	1.217433	-0.321838
6	6	0.664303	0.300998	-0.231867
7	8	0.584713	-0.932484	-0.251927
8	7	1.875422	0.949121	-0.121352
9	1	2.721892	0.336862	-0.066521
10	6	2.028297	2.322269	-0.063512
11	7	3.271478	2.768335	0.052767
12	1	4.085050	2.136054	0.095012
13	1	3.402707	3.768511	0.098024
14	7	1.017420	3.191930	-0.115730
15	6	-0.178384	2.619816	-0.252281
16	6	-1.635996	4.646929	-0.214713

17	1	-0.706071	5.181827	-0.403231
18	1	-2.387609	4.927583	-0.952379
19	1	-1.997588	4.880526	0.789933
20	7	6.544348	-0.932313	0.103852
21	6	6.495005	-2.288176	0.023818
22	1	7.449481	-2.801420	0.046403
23	6	5.316101	-2.949056	-0.077833
24	1	5.279237	-4.027597	-0.142764
25	6	4.127834	-2.151060	-0.096268
26	7	2.926377	-2.727356	-0.192999
27	1	2.084904	-2.155012	-0.209616
28	1	2.842601	-3.730176	-0.253628
29	7	4.178686	-0.816594	-0.018124
30	6	5.371952	-0.180094	0.080870
31	8	5.466031	1.057507	0.153237
32	6	7.814074	-0.214176	0.213004
33	1	7.932345	0.456543	-0.638731
34	1	7.826797	0.372221	1.132229
35	1	8.622017	-0.943503	0.226584
36	7	-5.619131	-1.893957	-0.075109
37	6	-5.227149	-3.194862	0.014111
38	1	-6.026736	-3.918367	0.120436
39	6	-3.924310	-3.575213	-0.022680
40	1	-3.641037	-4.614823	0.054520

41	6	-2.941878	-2.554476	-0.156305
42	7	-1.643235	-2.785818	-0.175795
43	1	-0.946139	-2.037653	-0.243929
44	1	-1.308338	-3.735210	-0.088439
45	7	-3.376003	-1.279531	-0.269840
46	6	-4.691961	-0.882370	-0.212566
47	8	-5.019348	0.296999	-0.282440
48	6	-7.031671	-1.498763	-0.024619
49	1	-7.198573	-0.856768	0.840366
50	1	-7.287238	-0.957292	-0.935249
51	1	-7.635202	-2.399949	0.056104
52	1	-2.690259	-0.484218	-0.331987
53	8	-3.473041	2.495811	-1.073229
54	1	-4.165521	1.842833	-0.849515
55	8	-3.081585	1.584505	2.160163
56	8	-2.747886	0.376276	2.008317

41. Int20

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.466404	3.340291	-0.100918
2	6	-2.395447	2.386098	0.188707
3	1	-2.149239	0.575802	2.033273
4	7	-1.873979	1.194792	0.415864
5	6	-0.504296	1.384879	0.228075
6	6	0.567112	0.464525	0.235594

7	8	0.504752	-0.769629	0.419383
8	7	1.788464	1.079187	-0.010098
9	1	2.620163	0.452941	-0.014280
10	6	1.954561	2.417620	-0.275757
11	7	3.207834	2.837460	-0.488252
12	1	4.008511	2.196567	-0.483836
13	1	3.340543	3.813161	-0.705448
14	7	0.945617	3.279840	-0.328857
15	6	-0.239856	2.708854	-0.077844
16	6	-1.732851	4.739935	-0.400889
17	1	-0.837602	5.153459	-0.862980
18	1	-2.572392	4.804317	-1.092736
19	1	-1.962671	5.286651	0.514785
20	7	6.431344	-0.956856	-0.276722
21	6	6.347118	-2.293878	-0.047645
22	1	7.281834	-2.842072	-0.077535
23	6	5.158987	-2.896256	0.202424
24	1	5.093827	-3.960204	0.383526
25	6	3.999227	-2.056146	0.214297
26	7	2.790505	-2.572154	0.454874
27	1	1.967673	-1.968053	0.458765
28	1	2.684162	-3.558128	0.635852
29	7	4.083791	-0.741194	-0.013171
30	6	5.284665	-0.162129	-0.261608

31	8	5.409540	1.054812	-0.477864
32	6	7.711124	-0.302153	-0.545220
33	1	7.683324	0.172857	-1.526492
34	1	7.901784	0.458654	0.212489
35	1	8.496311	-1.055749	-0.519811
36	7	-5.567542	-1.709111	-0.731577
37	6	-5.131968	-2.982583	-0.953289
38	1	-5.898366	-3.694972	-1.234510
39	6	-3.831515	-3.347842	-0.828088
40	1	-3.516487	-4.366351	-1.003142
41	6	-2.893295	-2.346402	-0.445579
42	7	-1.609702	-2.569296	-0.267525
43	1	-0.956271	-1.842214	0.057137
44	1	-1.247913	-3.502924	-0.406455
45	7	-3.369532	-1.090147	-0.265741
46	6	-4.686281	-0.717063	-0.375700
47	8	-5.055581	0.437968	-0.167901
48	6	-6.981710	-1.334816	-0.856503
49	1	-7.338227	-0.946944	0.097561
50	1	-7.087470	-0.569557	-1.625276
51	1	-7.544438	-2.223440	-1.132619
52	1	-2.727506	-0.310561	0.005267
53	8	-3.671316	2.705895	0.216184
54	1	-4.215013	1.877022	0.166331

55	8	-2.191395	-0.023380	2.837657
56	8	-2.033596	-1.227645	2.347435

42. C-8-OHG-C

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.575739	3.316441	-0.031433
2	6	-2.526098	2.330368	-0.035218
3	7	-2.025324	1.118544	-0.034536
4	6	-0.650036	1.319531	-0.028677
5	6	0.421599	0.402505	-0.025633
6	8	0.351992	-0.847542	-0.029567
7	7	1.659325	1.031168	-0.017850
8	1	2.489106	0.403613	-0.011225
9	6	1.847167	2.392775	-0.017055
10	7	3.117143	2.823873	-0.025119
11	1	3.911287	2.181062	0.056308
12	1	3.267647	3.819416	0.028918
13	7	0.847374	3.263818	-0.021305
14	6	-0.358779	2.675728	-0.027053
15	6	-1.824701	4.749765	-0.030349
16	1	-0.856899	5.248998	-0.013501
17	1	-2.371241	5.034403	-0.930337
18	1	-2.398640	5.027114	0.854663
19	7	6.318259	-0.994428	0.062103
20	6	6.219456	-2.345311	-0.049453

21	1	7.155833	-2.891397	-0.062066
22	6	5.016177	-2.962847	-0.138403
23	1	4.940042	-4.037713	-0.226663
24	6	3.856177	-2.123381	-0.106259
25	7	2.631817	-2.653542	-0.180690
26	1	1.809985	-2.049534	-0.136594
27	1	2.511576	-3.651872	-0.252732
28	7	3.955543	-0.794114	-0.001788
29	6	5.171546	-0.199551	0.082636
30	8	5.310231	1.030995	0.179586
31	6	7.614300	-0.324570	0.161274
32	1	7.738294	0.365274	-0.674287
33	1	7.668644	0.235477	1.095435
34	1	8.396067	-1.081774	0.136985
35	7	-5.824955	-1.761969	0.052928
36	6	-5.418820	-3.063108	0.071412
37	1	-6.212048	-3.800645	0.098363
38	6	-4.111057	-3.421916	0.057051
39	1	-3.815248	-4.460980	0.071105
40	6	-3.136778	-2.382428	0.022700
41	7	-1.838781	-2.604270	0.008492
42	1	-1.131000	-1.853057	-0.011641
43	1	-1.506912	-3.558913	0.023715
44	7	-3.582931	-1.103784	0.004488

45	6	-4.905352	-0.739853	0.019216
46	8	-5.258162	0.440077	0.003418
47	6	-7.244101	-1.386828	0.068981
48	1	-7.450685	-0.787412	0.955556
49	1	-7.475559	-0.808131	-0.825074
50	1	-7.836716	-2.298543	0.087721
51	1	-2.901743	-0.272380	-0.015328
52	8	-3.800207	2.672545	-0.038341
53	1	-4.358943	1.850951	-0.028153

43. C-8-oxoG-C

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	7	-1.991946	3.878598	-0.043514
2	6	-3.071415	3.029397	0.222822
3	6	-1.159295	1.836858	0.221900
4	6	-0.137363	0.889591	0.285398
5	8	-0.241158	-0.350534	0.527345
6	7	1.118366	1.422925	0.052654
7	1	1.915415	0.749209	0.127241
8	6	1.359581	2.742468	-0.208825
9	7	2.641244	3.102466	-0.385201
10	1	3.360811	2.392744	-0.549282
11	1	2.808990	4.051526	-0.683830
12	7	0.395267	3.655185	-0.267432
13	6	-0.827161	3.161385	-0.045996

14	6	-2.145500	5.302138	-0.279690
15	1	-1.159111	5.714152	-0.487736
16	1	-2.803479	5.466890	-1.134460
17	1	-2.568698	5.783688	0.603481
18	7	5.498604	-0.961159	-0.221639
19	6	5.414224	-2.154828	0.421770
20	1	6.309509	-2.765770	0.409168
21	6	4.273445	-2.550228	1.039740
22	1	4.208901	-3.501786	1.548934
23	6	3.162952	-1.650827	0.975697
24	7	1.995072	-1.967077	1.549396
25	1	1.203199	-1.334140	1.466436
26	1	1.887170	-2.832483	2.055560
27	7	3.248836	-0.477014	0.344841
28	6	4.403427	-0.098694	-0.260202
29	8	4.522137	0.988248	-0.847629
30	6	6.728742	-0.530345	-0.885348
31	1	6.531948	-0.352013	-1.942942
32	1	7.088872	0.392831	-0.429947
33	1	7.474088	-1.315768	-0.773158
34	7	-4.410512	-2.822256	-0.219444
35	6	-3.879750	-3.942272	-0.780284
36	1	-4.592703	-4.713291	-1.047414
37	6	-2.547862	-4.098559	-1.001679

38	1	-2.153996	-4.996827	-1.453772
39	6	-1.692953	-3.031637	-0.617564
40	7	-0.380718	-3.038739	-0.773947
41	1	0.177443	-2.234431	-0.499957
42	1	0.081777	-3.838015	-1.183404
43	7	-2.258112	-1.940081	-0.053728
44	6	-3.606616	-1.764972	0.158471
45	8	-4.056717	-0.738292	0.649184
46	6	-5.853740	-2.668980	-0.000595
47	1	-6.040820	-2.490815	1.058138
48	1	-6.221436	-1.824493	-0.583609
49	1	-6.345240	-3.585843	-0.317707
50	1	-1.609218	-1.168745	0.254969
51	8	-4.245997	3.377451	0.283971
52	7	-2.541377	1.778298	0.392665
53	1	-3.106916	0.947406	0.564067