Electronic Supplementary Material (ESI) for RSC Advances

Supplementary data

Enantioselectivity of aza-MBH-type reaction of nitroalkene to N-tosylimine catalyzed by thiourea-tertiary amine: a theoretical study

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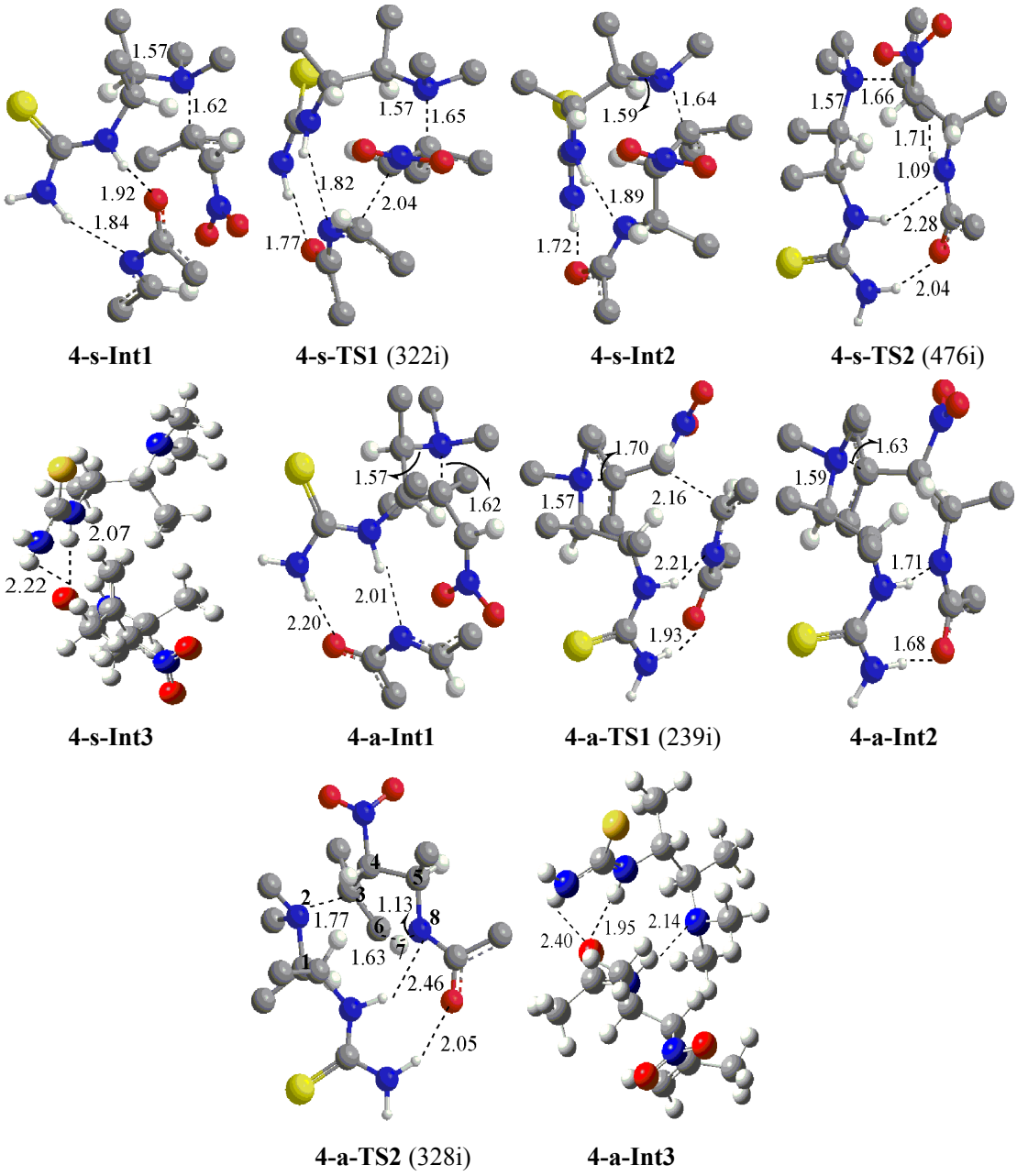
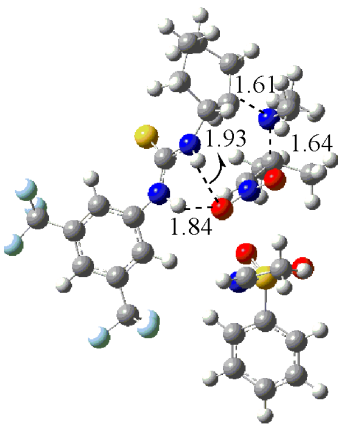
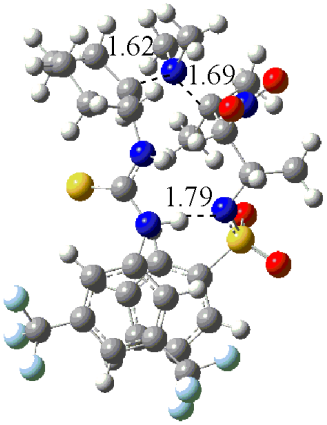
Figure 1. Optimized structure and selected geometric parameters of species with catalyst model **4** and of Ints with full catalyst **5**.

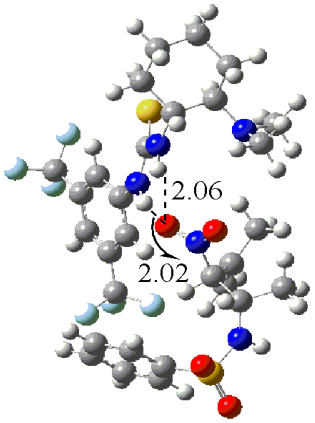




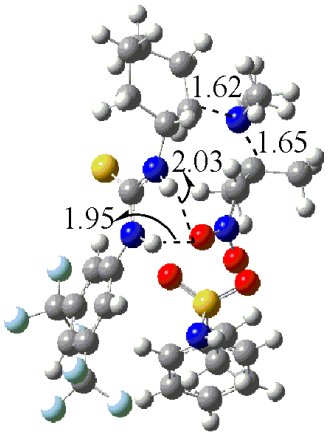
5-s-Int1



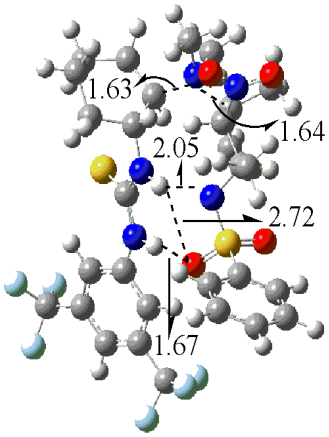
5-s-Int2



5-s-Int3



5-a-Int1



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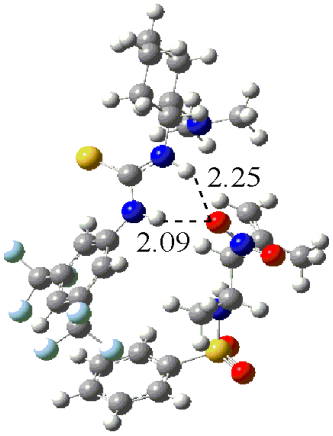
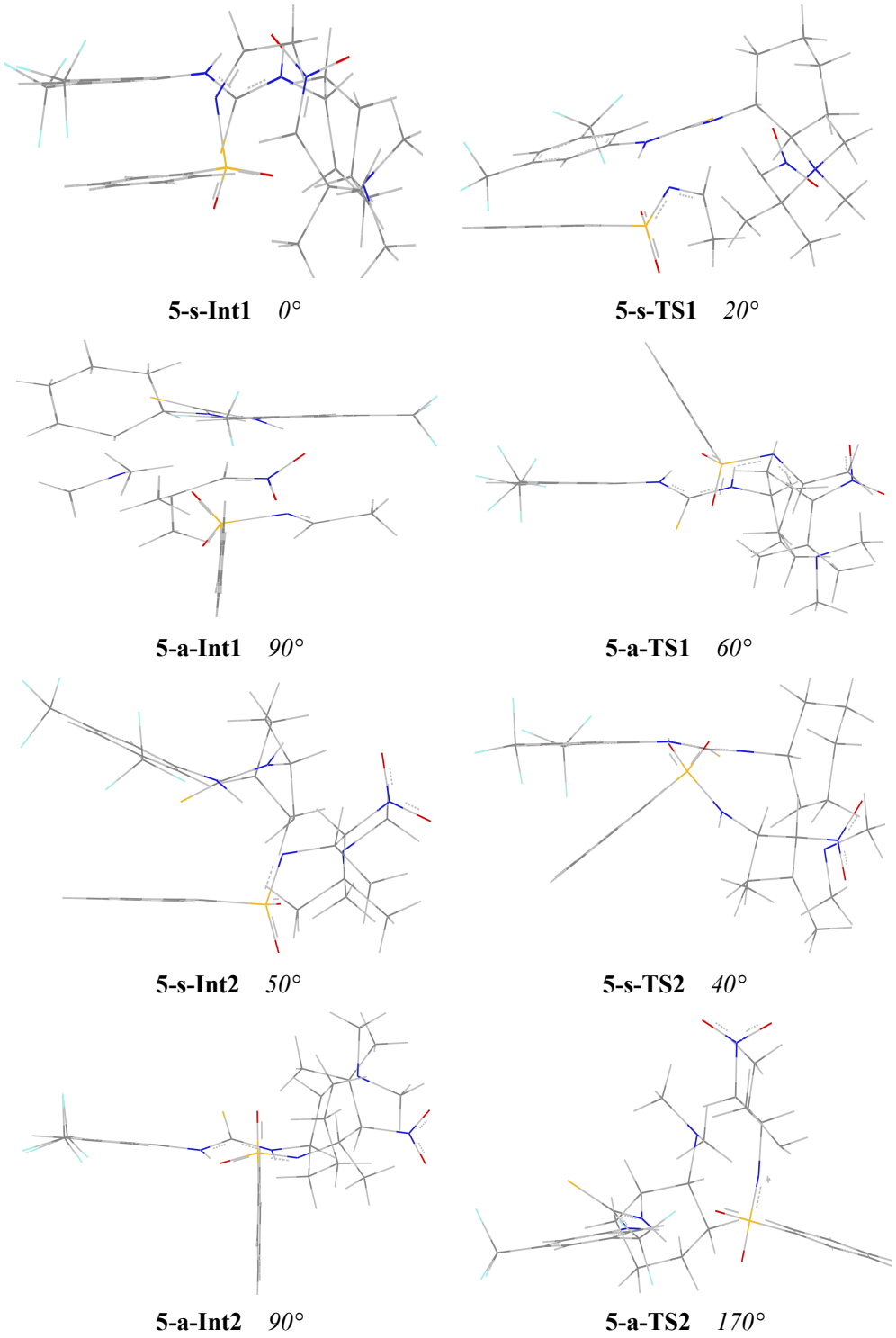


5-a-Int3

Figure 2. The π-π aromatic stacking interaction of related species in two steps of the aza-MBH-type reaction with full catalyst **5**. The approximate angles between two planes of aromatic ring are given in italic.



5-s-Int1 *0°* **5-s-TS1** *20°*

5-a-Int1 *90°* **5-a-TS1** *60°*

5-s-Int2 *50°* **5-s-TS2** *40°*

5-a-Int2 *90°* **5-a-TS2** *170°*

Table 1. Atom coordinates and two energies of **4-s-Int1** (E= -1486.9188 a.u., G= -1487.0031 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.016565	-0.021490	-0.008617
2	6	0	-0.098414	-0.067933	1.547557
3	7	0	1.209748	-0.044085	2.172394
4	6	0	2.198224	-0.939928	2.057637
5	7	0	3.238180	-0.717061	2.871735
6	16	0	2.213138	-2.237138	0.967002
7	7	0	-0.353026	1.392680	-0.598274
8	6	0	-0.364393	1.272618	-2.087162
9	6	0	-1.736598	1.804066	-0.225176
10	6	0	0.730611	2.528839	-0.207629
11	6	0	0.444926	2.984430	1.198349
12	6	0	2.128426	1.937118	-0.395523
13	6	0	0.595447	3.730888	-1.155697
14	7	0	1.255950	3.817914	1.828023
15	8	0	2.362690	4.170549	1.322487
16	8	0	0.927697	4.266641	2.959564
17	1	0	1.010367	-0.182307	-0.289965
18	1	0	-0.525086	0.863311	1.884438
19	1	0	1.251242	0.582269	2.969793
20	1	0	3.298846	0.114667	3.440864
21	1	0	4.022100	-1.328238	2.791838
22	1	0	-0.596021	2.231626	-2.519271
23	1	0	-1.125315	0.570593	-2.384044
24	1	0	0.598478	0.931941	-2.437755
25	1	0	-1.902424	2.824244	-0.539147
26	1	0	-1.892893	1.732649	0.837374
27	1	0	-2.439863	1.155015	-0.728493
28	1	0	-0.514742	2.915032	1.659395
29	1	0	2.261593	1.490090	-1.376208
30	1	0	2.371657	1.215991	0.370424
31	1	0	2.821185	2.758137	-0.293405
32	1	0	1.220806	4.493523	-0.704827
33	1	0	-0.414323	4.125410	-1.211598
34	1	0	0.971125	3.546246	-2.157677
35	6	0	3.630852	3.176712	3.675983
36	7	0	3.061701	2.169987	4.199693
37	6	0	4.965214	3.072324	3.035878
38	1	0	3.139412	4.140610	3.624061

39	1	0	5.369611	2.070226	3.118254
40	1	0	4.861287	3.351856	1.991194
41	1	0	5.652363	3.782956	3.491316
42	6	0	-0.970528	-1.173362	2.144100
43	1	0	-0.548361	-2.155577	1.972324
44	1	0	-1.022589	-1.009374	3.215563
45	1	0	-1.984010	-1.145141	1.753217
46	6	0	-0.827520	-1.122348	-0.681471
47	1	0	-0.544895	-2.047054	-0.198005
48	1	0	-1.902554	-1.002774	-0.587124
49	1	0	-0.574182	-1.243248	-1.726425
50	6	0	1.799569	2.305265	4.797243
51	8	0	0.928965	1.510769	4.525188
52	6	0	1.625262	3.354589	5.852210
53	1	0	2.442275	3.320687	6.566539
54	1	0	1.621440	4.326575	5.368227
55	1	0	0.678787	3.203267	6.354136

Table 2. Atom coordinates and two energies of **4-s-TS1** (E= -1486.8952 a.u., G= -1486.9746 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.001558	-0.000473	0.000365
2	6	0	0.003689	-0.000702	1.568479
3	7	0	1.358411	0.000148	2.098181
4	6	0	2.288203	-0.968058	1.929062
5	7	0	3.485299	-0.687625	2.438216
6	16	0	2.006290	-2.427767	1.115649
7	1	0	1.013285	-0.173756	-0.322458
8	1	0	-0.411949	0.935168	1.900905
9	1	0	1.667194	0.840870	2.568409
10	1	0	3.783149	0.274611	2.612021
11	1	0	4.194768	-1.368925	2.263816
12	7	0	-0.367596	1.383500	-0.636566
13	6	0	-0.376392	1.199081	-2.114466
14	6	0	-1.744433	1.792728	-0.252175
15	6	0	0.706729	2.649396	-0.270622
16	6	0	0.378745	3.188148	1.088957
17	6	0	2.108778	2.056479	-0.307265
18	6	0	0.626691	3.685327	-1.393407
19	7	0	-0.717562	4.063951	1.264539
20	8	0	-1.024115	4.883781	0.402152

21	8	0	-1.268070	4.030697	2.358922
22	6	0	1.795380	4.068428	2.258784
23	7	0	2.588093	3.070385	2.634342
24	1	0	-0.629767	2.129641	-2.593057
25	1	0	-1.121862	0.469435	-2.385633
26	1	0	0.594626	0.860471	-2.449947
27	1	0	-1.956506	2.768192	-0.666770
28	1	0	-1.845436	1.845491	0.820864
29	1	0	-2.450860	1.073276	-0.642745
30	1	0	0.312454	2.452356	1.853614
31	1	0	2.808499	2.883907	-0.291775
32	1	0	2.283034	1.514471	-1.231182
33	1	0	1.149256	4.565819	-1.042862
34	1	0	-0.372412	4.013832	-1.636418
35	1	0	1.135064	3.329813	-2.282284
36	1	0	2.346839	1.425505	0.531382
37	6	0	-0.878115	-1.047805	2.251035
38	1	0	-0.524103	-2.055457	2.087633
39	1	0	-0.857686	-0.850060	3.317770
40	1	0	-1.908727	-0.964192	1.917660
41	6	0	-0.845507	-1.129741	-0.583161
42	1	0	-1.913280	-1.001910	-0.438452
43	1	0	-0.646833	-1.297042	-1.633401
44	1	0	-0.537042	-2.031418	-0.073276
45	6	0	3.924419	2.982087	2.529782
46	8	0	4.491129	1.889727	2.489262
47	6	0	4.826574	4.203950	2.585399
48	1	0	4.977147	4.617747	1.591867
49	1	0	4.427600	4.985318	3.221752
50	1	0	5.790318	3.884772	2.961205
51	6	0	2.206448	5.304485	1.496189
52	1	0	2.889438	5.084747	0.682673
53	1	0	1.331550	5.809505	1.101082
54	1	0	2.705993	5.996822	2.169622
55	1	0	0.977415	4.267570	2.942272

Table 3. Atom coordinates and two energies of **4-s-Int2** (E= -1486.9015 a.u., G= -1486.9794 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.122538	-0.093528	0.074576
2	6	0	0.156651	0.169356	1.593588

3	7	0	1.529137	-0.104528	1.951195
4	6	0	2.151882	-1.301719	1.868206
5	7	0	3.428554	-1.275728	2.218755
6	16	0	1.413381	-2.732023	1.307157
7	1	0	0.718331	-0.645667	-0.311764
8	1	0	0.036590	1.226283	1.780669
9	1	0	2.156654	0.710486	1.999282
10	1	0	3.889798	-0.416902	2.563838
11	1	0	3.927324	-2.138232	2.161648
12	7	0	-0.150709	1.221458	-0.816300
13	6	0	-0.531886	0.787124	-2.196001
14	6	0	-1.246600	2.125539	-0.370879
15	6	0	1.275190	2.019080	-0.916939
16	6	0	1.455717	2.940518	0.330589
17	6	0	2.373464	0.961777	-1.022958
18	6	0	1.313518	2.820995	-2.222501
19	7	0	0.725952	4.257882	0.237976
20	8	0	1.009146	5.039089	-0.640152
21	8	0	-0.068338	4.493484	1.122489
22	6	0	2.890562	3.280645	0.877160
23	7	0	3.302517	2.093593	1.556847
24	1	0	-0.584461	1.642362	-2.847390
25	1	0	-1.506898	0.332635	-2.162790
26	1	0	0.184915	0.071492	-2.572263
27	1	0	-1.280895	2.993260	-1.016570
28	1	0	-1.103941	2.449924	0.645702
29	1	0	-2.184856	1.595666	-0.450073
30	1	0	0.996033	2.494062	1.186629
31	1	0	3.280738	1.454107	-1.340626
32	1	0	2.123925	0.238268	-1.791897
33	1	0	2.174754	3.471797	-2.173544
34	1	0	0.458149	3.463111	-2.388673
35	1	0	1.448657	2.164536	-3.072558
36	1	0	2.598168	0.468376	-0.094904
37	6	0	-0.823131	-0.476673	2.575753
38	1	0	-0.745146	-1.555005	2.574116
39	1	0	-0.566875	-0.121357	3.568036
40	1	0	-1.848418	-0.182976	2.368250
41	6	0	-1.353697	-0.960106	-0.162055
42	1	0	-2.295772	-0.477303	0.078032
43	1	0	-1.401056	-1.360241	-1.165968
44	1	0	-1.234363	-1.814532	0.489443
45	6	0	4.211748	2.111709	2.516179
46	8	0	4.559008	1.069435	3.103974

47	6	0	4.906431	3.384279	2.976150
48	1	0	5.853360	3.487837	2.451153
49	1	0	4.332357	4.291992	2.816898
50	1	0	5.128767	3.280982	4.031095
51	6	0	3.885618	3.840389	-0.140782
52	1	0	4.241961	3.080604	-0.826791
53	1	0	3.472698	4.673545	-0.701569
54	1	0	4.753066	4.206705	0.396704
55	1	0	2.674035	4.104386	1.568546

Table 4. Atom coordinates and two energies of **4-s-TS2** (E= -1486.8685 a.u., G= -1486.9490 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.004107	-0.007581	-0.001850
2	6	0	0.001170	-0.001508	1.558879
3	7	0	1.375988	0.002122	2.035082
4	6	0	2.255539	-0.985696	2.292944
5	7	0	3.420590	-0.528508	2.768690
6	16	0	2.030162	-2.647478	2.074797
7	1	0	0.940237	0.424899	-0.287812
8	1	0	-0.351796	0.961892	1.889160
9	1	0	1.764286	0.923876	2.165570
10	1	0	3.570450	0.453476	2.928505
11	1	0	4.130178	-1.197479	2.974648
12	7	0	-1.028955	0.986226	-0.671167
13	6	0	-1.163253	0.583749	-2.104004
14	6	0	-2.388677	0.821922	-0.096518
15	6	0	-0.510761	2.559584	-0.664840
16	6	0	-0.884212	3.215575	0.725504
17	6	0	0.996300	2.515735	-0.826074
18	6	0	-1.222478	3.305582	-1.798903
19	7	0	-2.226576	3.900699	0.756425
20	8	0	-2.357067	4.971390	0.213517
21	8	0	-3.109263	3.344806	1.375950
22	6	0	0.163519	4.160549	1.397543
23	7	0	1.281248	3.286728	1.668312
24	1	0	-1.901586	1.205370	-2.581836
25	1	0	-1.499402	-0.438317	-2.153684
26	1	0	-0.211111	0.685140	-2.603258
27	1	0	-3.078996	1.472405	-0.615919
28	1	0	-2.411254	1.067082	0.950744

29	1	0	-2.698991	-0.205994	-0.232502
30	1	0	-1.026602	2.446808	1.457831
31	1	0	1.290612	3.501436	-1.182868
32	1	0	1.255243	1.845962	-1.645959
33	1	0	-0.991882	4.354991	-1.670308
34	1	0	-2.308987	3.228843	-1.814283
35	1	0	-0.821833	3.008795	-2.757920
36	1	0	1.495749	2.719882	0.719245
37	6	0	-0.882605	-1.034448	2.250791
38	1	0	-0.588574	-2.048509	2.026576
39	1	0	-0.797065	-0.901501	3.324231
40	1	0	-1.924093	-0.893152	1.978884
41	6	0	-0.106629	-1.423296	-0.547182
42	1	0	-1.097740	-1.859472	-0.448718
43	1	0	0.214401	-1.501145	-1.578256
44	1	0	0.570962	-2.031101	0.044918
45	6	0	2.019027	3.250741	2.779185
46	8	0	2.876779	2.381743	2.941584
47	6	0	1.768253	4.259082	3.877349
48	1	0	1.697638	5.274491	3.501036
49	1	0	0.838053	4.030363	4.393324
50	1	0	2.579306	4.190256	4.589757
51	6	0	0.556925	5.442723	0.668497
52	1	0	1.034155	5.240090	-0.280963
53	1	0	-0.298303	6.085797	0.504805
54	1	0	1.274026	5.976640	1.284903
55	1	0	-0.309681	4.455015	2.333815

Table 5. Atom coordinates and two energies of **4-s-Int3** (E= -1486.9427 a.u., G= -1487.0374 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.023864	0.001406	-0.002516
2	6	0	0.015520	-0.003677	1.540652
3	7	0	1.369396	-0.012996	2.077699
4	6	0	2.132765	1.063343	2.271141
5	7	0	3.368411	0.789321	2.791284
6	16	0	1.711927	2.641381	1.883620
7	1	0	0.611658	0.876452	-0.264437
8	1	0	-0.432543	0.937938	1.836220
9	1	0	1.781898	-0.904732	2.303682
10	1	0	3.485978	-0.081580	3.281164

11	1	0	3.846326	1.588326	3.156496
12	7	0	-1.335476	0.244441	-0.493373
13	6	0	-1.431250	1.387211	-1.372955
14	6	0	-2.065175	-0.887524	-1.014373
15	6	0	6.813316	0.907253	0.315982
16	6	0	6.839566	-0.575513	0.046605
17	6	0	5.723331	1.658327	0.274778
18	6	0	8.138712	1.475133	0.742096
19	7	0	7.770157	-0.897043	-1.103011
20	8	0	7.967597	-0.055528	-1.943126
21	8	0	8.223207	-2.018781	-1.117576
22	6	0	5.545309	-1.371155	-0.240794
23	6	0	4.827350	-1.010537	-1.538891
24	7	0	4.680737	-1.317224	0.917501
25	1	0	-2.477447	1.614222	-1.562625
26	1	0	-0.944357	1.232805	-2.345025
27	1	0	-0.982391	2.255984	-0.902576
28	1	0	-3.107172	-0.605755	-1.143333
29	1	0	-2.039718	-1.721091	-0.321383
30	1	0	-1.699984	-1.245329	-1.984498
31	1	0	7.319423	-1.068319	0.886839
32	1	0	5.770779	2.701467	0.539405
33	1	0	4.750872	1.302177	-0.008514
34	1	0	8.878031	1.382173	-0.048486
35	1	0	8.525444	0.952580	1.616129
36	1	0	8.045160	2.525813	0.991379
37	1	0	5.887451	-2.393556	-0.338332
38	1	0	4.409483	-0.012364	-1.526405
39	1	0	4.014286	-1.711860	-1.698010
40	1	0	5.501378	-1.078159	-2.386732
41	1	0	4.382828	-0.415212	1.256483
42	6	0	-0.767959	-1.140687	2.174724
43	1	0	-0.351461	-2.115333	1.927504
44	1	0	-0.764119	-1.041593	3.256198
45	1	0	-1.797162	-1.110432	1.837255
46	6	0	0.733573	-1.202130	-0.618977
47	1	0	0.250930	-2.146383	-0.384581
48	1	0	0.771613	-1.109821	-1.701006
49	1	0	1.756593	-1.252155	-0.257716
50	6	0	4.167277	-2.358792	1.606580
51	8	0	3.403130	-2.172338	2.544780
52	6	0	4.553406	-3.757815	1.202874
53	1	0	5.625060	-3.914457	1.288664
54	1	0	4.039925	-4.442565	1.863264

55	1	0	4.266857	-3.967654	0.176216

Table 6. Atom coordinates and two energies of **4-a-Int1** (E= -1486.9165 a.u., G= -1487.0003 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.007869	0.007289	0.003181
2	6	0	0.011052	0.003075	1.565364
3	7	0	1.354411	-0.004555	2.117689
4	6	0	2.309764	-0.938925	1.966996
5	7	0	3.436252	-0.694228	2.641166
6	16	0	2.168172	-2.320544	0.995917
7	7	0	-0.515355	1.359797	-0.596949
8	6	0	-0.428751	1.255766	-2.083361
9	6	0	-1.962111	1.528348	-0.279444
10	6	0	0.337760	2.662528	-0.145471
11	6	0	-0.146906	3.075334	1.220067
12	6	0	1.820530	2.302679	-0.215769
13	6	0	0.085182	3.818976	-1.124630
14	7	0	0.467121	4.022111	1.918573
15	8	0	1.573678	4.497773	1.553670
16	8	0	-0.066417	4.442695	2.980967
17	1	0	1.032111	-0.043546	-0.329494
18	1	0	-0.355885	0.970174	1.879194
19	1	0	1.530864	0.718116	2.810173
20	1	0	3.626116	0.211383	3.051973
21	1	0	4.191809	-1.328476	2.491091
22	1	0	-0.839067	2.147399	-2.528244
23	1	0	-1.004556	0.409972	-2.418518
24	1	0	0.601345	1.133335	-2.383699
25	1	0	-2.267101	2.538371	-0.511615
26	1	0	-2.146170	1.329357	0.764188
27	1	0	-2.536800	0.835841	-0.877686
28	1	0	-1.163086	2.946918	1.522822
29	1	0	2.097632	1.913536	-1.191323
30	1	0	2.113533	1.601089	0.550823
31	1	0	2.369830	3.214902	-0.039713
32	1	0	0.553370	4.674844	-0.650478
33	1	0	-0.967493	4.052260	-1.254094
34	1	0	0.550523	3.685670	-2.096499
35	6	0	0.960276	2.853234	4.756295
36	7	0	1.854839	2.190526	4.138636

37	6	0	-0.371036	2.271305	5.054766
38	1	0	1.135062	3.854401	5.127372
39	1	0	-0.427702	1.240200	4.725994
40	1	0	-0.568789	2.318682	6.123720
41	1	0	-1.118180	2.874391	4.548507
42	6	0	-0.722981	-1.187496	-0.599084
43	1	0	-1.795722	-1.174609	-0.439144
44	1	0	-0.522387	-1.312053	-1.655200
45	1	0	-0.313974	-2.062379	-0.113191
46	6	0	-0.876794	-1.048425	2.230151
47	1	0	-0.503783	-2.051794	2.070550
48	1	0	-0.883836	-0.860112	3.299206
49	1	0	-1.903542	-0.989847	1.877828
50	6	0	3.116671	2.772968	3.904290
51	8	0	3.989189	2.054389	3.473628
52	6	0	3.361979	4.232329	4.158880
53	1	0	2.672271	4.816969	3.555976
54	1	0	3.220012	4.480019	5.207731
55	1	0	4.383066	4.454026	3.879812

Table 7. Atom coordinates and two energies of **4-a-TS1** (E= -1486.8902 a.u., G= -1486.9699 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.005628	-0.002076	0.000663
2	6	0	0.003750	0.001373	1.561769
3	7	0	1.345452	0.000962	2.105314
4	6	0	2.329033	-0.896310	1.937560
5	7	0	3.481204	-0.549626	2.520841
6	16	0	2.191987	-2.342338	1.063749
7	1	0	1.022573	-0.005719	-0.329812
8	1	0	-0.373080	0.960085	1.880756
9	1	0	1.532658	0.821432	2.691149
10	1	0	3.642950	0.413367	2.795395
11	1	0	4.260143	-1.153048	2.363084
12	7	0	-0.590880	1.317501	-0.627062
13	6	0	-0.362306	1.205492	-2.100664
14	6	0	-2.071255	1.361138	-0.438990
15	6	0	0.101434	2.726313	-0.116541
16	6	0	-0.584942	3.160948	1.197489
17	6	0	1.601056	2.493685	-0.004011
18	6	0	-0.110428	3.766285	-1.223167

19	7	0	-1.100044	4.480107	1.259451
20	8	0	-0.367216	5.434196	1.004961
21	8	0	-2.228637	4.630799	1.714249
22	6	0	0.420989	3.323713	3.108018
23	7	0	1.509346	2.574573	3.189952
24	1	0	-0.881726	1.998696	-2.611613
25	1	0	-0.753740	0.266503	-2.449536
26	1	0	0.695691	1.251709	-2.313903
27	1	0	-2.430682	2.366565	-0.604839
28	1	0	-2.338665	1.049942	0.559111
29	1	0	-2.534366	0.689834	-1.148166
30	1	0	-1.396339	2.529587	1.490300
31	1	0	2.043112	3.451479	0.246707
32	1	0	2.033777	2.185423	-0.951293
33	1	0	0.250790	4.707958	-0.840662
34	1	0	-1.154256	3.914940	-1.484199
35	1	0	0.457441	3.534714	-2.113709
36	1	0	1.886155	1.791343	0.760089
37	6	0	-0.882165	-1.042969	2.242010
38	1	0	-0.505991	-2.046014	2.090239
39	1	0	-0.877689	-0.842167	3.308411
40	1	0	-1.911950	-0.990910	1.897368
41	6	0	-0.682848	-1.241719	-0.574924
42	1	0	-1.750025	-1.280146	-0.388946
43	1	0	-0.500764	-1.380992	-1.632153
44	1	0	-0.216104	-2.083275	-0.081114
45	6	0	2.742990	3.091166	2.941380
46	8	0	3.704408	2.344851	2.804351
47	6	0	2.973052	4.587867	2.878759
48	1	0	2.370645	5.062288	2.108677
49	1	0	2.709634	5.054909	3.824296
50	1	0	4.021033	4.762004	2.675825
51	6	0	-0.742860	2.909021	3.961460
52	1	0	-0.513935	3.206970	4.983612
53	1	0	-1.667884	3.390233	3.669998
54	1	0	-0.857802	1.829767	3.963429
55	1	0	0.514022	4.394050	2.965884

Table 8. Atom coordinates and two energies of **4-a-Int2** (E= -1486.9054 a.u., G= -1486.9839 a.u.)

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

1	6	0	0.008180	-0.154234	0.030174
2	6	0	-0.043239	-0.164335	1.595734
3	7	0	1.275640	-0.230384	2.181782
4	6	0	2.160926	-1.240555	2.033887
5	7	0	3.334519	-1.037534	2.612270
6	16	0	1.855120	-2.660353	1.140488
7	1	0	1.020375	-0.385460	-0.259018
8	1	0	-0.426795	0.789230	1.921871
9	1	0	1.647605	0.664710	2.529291
10	1	0	3.600953	-0.132240	3.035540
11	1	0	4.020620	-1.751277	2.485053
12	7	0	-0.245048	1.276336	-0.612166
13	6	0	-0.229087	1.077923	-2.095069
14	6	0	-1.620097	1.747171	-0.288840
15	6	0	0.868147	2.409885	-0.244417
16	6	0	0.549382	3.066455	1.143165
17	6	0	2.239065	1.736052	-0.277925
18	6	0	0.898929	3.471925	-1.351574
19	7	0	-0.464143	4.181402	1.047161
20	8	0	-0.169468	5.194758	0.458414
21	8	0	-1.507557	4.022253	1.641037
22	6	0	1.760330	3.592779	1.975997
23	7	0	2.370190	2.411473	2.507352
24	1	0	-0.416923	2.014328	-2.591273
25	1	0	-1.014355	0.393121	-2.364157
26	1	0	0.723120	0.671442	-2.404584
27	1	0	-1.793351	2.704755	-0.760725
28	1	0	-1.760897	1.850691	0.773507
29	1	0	-2.330716	1.033586	-0.679325
30	1	0	0.065968	2.375974	1.803142
31	1	0	2.991351	2.508636	-0.183354
32	1	0	2.390952	1.259742	-1.241470
33	1	0	1.510195	4.288884	-0.993043
34	1	0	-0.063556	3.900741	-1.600557
35	1	0	1.365362	3.082841	-2.247024
36	1	0	2.409086	1.034930	0.518050
37	6	0	-1.007590	-1.168944	2.229945
38	1	0	-0.691716	-2.190636	2.072840
39	1	0	-1.016996	-0.979139	3.297964
40	1	0	-2.020110	-1.037226	1.857524
41	6	0	-0.880741	-1.218723	-0.601509
42	1	0	-1.944856	-1.037254	-0.491994
43	1	0	-0.651296	-1.396043	-1.643718
44	1	0	-0.637044	-2.137035	-0.085599

45	6	0	3.604370	2.425213	2.974350
46	8	0	4.141462	1.408931	3.457117
47	6	0	4.483018	3.669477	2.979914
48	1	0	5.486466	3.369777	2.699956
49	1	0	4.154784	4.475802	2.332642
50	1	0	4.537040	4.052284	3.995997
51	6	0	1.274845	4.524145	3.094237
52	1	0	0.833030	5.447363	2.732502
53	1	0	0.561188	4.006894	3.729309
54	1	0	2.127154	4.783491	3.710209
55	1	0	2.397950	4.175278	1.303469

Table 9. Atom coordinates and two energies of **4-a-TS2** (E= -1486.8666 a.u., G= -1486.9460 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.004013	0.007317	0.002953
2	6	0	-0.000493	0.007001	1.562114
3	7	0	1.376278	0.000077	2.039143
4	6	0	2.256721	-0.985058	2.300651
5	7	0	3.450983	-0.521284	2.695160
6	16	0	2.003872	-2.653883	2.194823
7	1	0	0.920334	0.509847	-0.281712
8	1	0	-0.344857	0.976900	1.891136
9	1	0	1.770042	0.923410	2.117145
10	1	0	3.650502	0.464284	2.714409
11	1	0	4.165559	-1.191471	2.878931
12	7	0	-1.059718	0.925695	-0.657370
13	6	0	-1.149943	0.539635	-2.091485
14	6	0	-2.416294	0.714583	-0.104491
15	6	0	-0.577848	2.625911	-0.650596
16	6	0	-0.991048	3.227754	0.750208
17	6	0	0.887196	2.632333	-0.824384
18	6	0	-1.375625	3.271027	-1.786554
19	7	0	-2.207683	4.097888	0.605040
20	8	0	-2.050676	5.263580	0.332745
21	8	0	-3.284914	3.568818	0.763778
22	6	0	0.061469	4.013662	1.577701
23	7	0	1.171005	3.095831	1.765065
24	1	0	-1.908394	1.129368	-2.578043
25	1	0	-1.434669	-0.497839	-2.168270
26	1	0	-0.194073	0.691460	-2.572522

27	1	0	-3.119571	1.355613	-0.616594
28	1	0	-2.459609	0.941263	0.947287
29	1	0	-2.700786	-0.321261	-0.250528
30	1	0	-1.347938	2.442622	1.391921
31	1	0	1.214866	3.670615	-0.788183
32	1	0	1.159091	2.255660	-1.809399
33	1	0	-1.199614	4.336794	-1.704722
34	1	0	-2.453833	3.120860	-1.770338
35	1	0	-0.978131	2.971819	-2.745199
36	1	0	1.330752	2.578280	0.824937
37	6	0	-0.882620	-1.029220	2.251161
38	1	0	-0.600842	-2.041753	2.005694
39	1	0	-0.776855	-0.917800	3.325255
40	1	0	-1.927295	-0.877368	2.000349
41	6	0	-0.000196	-1.414043	-0.542162
42	1	0	-0.969387	-1.902636	-0.468905
43	1	0	0.345290	-1.471397	-1.566893
44	1	0	0.691278	-1.991188	0.063199
45	6	0	2.320919	3.328278	2.440149
46	8	0	3.166704	2.442942	2.494758
47	6	0	2.599864	4.646726	3.117132
48	1	0	3.674505	4.776319	3.142995
49	1	0	2.140396	5.490259	2.613674
50	1	0	2.244898	4.620883	4.143825
51	6	0	-0.573945	4.421694	2.906634
52	1	0	0.122165	4.981334	3.516028
53	1	0	-1.440212	5.055739	2.757506
54	1	0	-0.871301	3.538724	3.466697
55	1	0	0.347895	4.904691	1.020521

Table 10. Atom coordinates and two energies of **4-a-Int3** (E= -1486.9446 a.u., G= -1487.0349 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.053036	-1.401255	0.361943
2	6	0	0.239377	-1.476498	1.866549
3	7	0	1.462948	-0.741557	2.129851
4	6	0	1.798372	-0.203527	3.303725
5	7	0	3.031356	0.366917	3.330906
6	16	0	0.808352	-0.158943	4.663156
7	1	0	0.843576	-1.755260	-0.146850
8	1	0	-0.556810	-0.997139	2.428352

9	1	0	2.096814	-0.597238	1.355832
10	1	0	3.694713	0.125414	2.618826
11	1	0	3.376980	0.600246	4.238276
12	7	0	-0.224477	-0.007803	-0.082627
13	6	0	0.057094	0.149275	-1.498687
14	6	0	-1.511971	0.567121	0.263823
15	6	0	0.549552	4.110959	-1.442289
16	6	0	0.490555	4.057694	0.069900
17	6	0	1.690235	4.090540	-2.111911
18	6	0	-0.784265	4.239660	-2.120111
19	7	0	0.232212	5.474492	0.529359
20	8	0	1.180831	6.218135	0.602281
21	8	0	-0.913377	5.776548	0.761454
22	6	0	1.696658	3.516311	0.848906
23	7	0	1.984728	2.158963	0.428202
24	1	0	0.025063	1.202445	-1.761536
25	1	0	-0.649484	-0.377702	-2.146977
26	1	0	1.059135	-0.210166	-1.710337
27	1	0	-1.509084	1.626126	0.021443
28	1	0	-1.698053	0.474685	1.328079
29	1	0	-2.349880	0.115709	-0.273925
30	1	0	-0.406458	3.532323	0.377609
31	1	0	1.698540	4.151381	-3.187605
32	1	0	2.647196	4.013155	-1.629299
33	1	0	-1.326179	5.110473	-1.759534
34	1	0	-1.411877	3.373647	-1.916060
35	1	0	-0.667325	4.328146	-3.194340
36	1	0	1.235154	1.472158	0.466402
37	6	0	0.374151	-2.912107	2.366748
38	1	0	1.114065	-3.458595	1.785176
39	1	0	0.689040	-2.897112	3.403554
40	1	0	-0.569869	-3.444306	2.313705
41	6	0	-1.205684	-2.321765	-0.043675
42	1	0	-2.085490	-2.167008	0.575294
43	1	0	-1.489992	-2.152768	-1.077850
44	1	0	-0.918399	-3.363147	0.045055
45	6	0	3.210966	1.610502	0.353241
46	8	0	3.359796	0.396643	0.255391
47	6	0	4.418754	2.511963	0.401013
48	1	0	4.506271	2.985104	1.375570
49	1	0	5.292290	1.899263	0.225277
50	1	0	4.378609	3.298038	-0.346153
51	6	0	1.444702	3.574036	2.355057
52	1	0	2.293366	3.155742	2.884407

53	1	0	1.296478	4.592804	2.697236
54	1	0	0.575881	2.980870	2.628012
55	1	0	2.544791	4.143029	0.607338

Table 11. Atom coordinates and two energies of **5-s-Int1** (E= -3095.9361 a.u., G= -3096.0627 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.684735	0.795423	-0.304808
2	6	0	-0.857171	0.787154	1.042490
3	7	0	0.301943	1.175385	1.680659
4	16	0	-2.255856	0.267622	1.829300
5	7	0	-0.865075	-2.288495	-1.823970
6	6	0	-1.533268	-3.634519	-2.008940
7	6	0	-0.476285	-1.815706	-3.208970
8	1	0	0.199992	1.165614	-0.626543
9	1	0	1.141448	1.130441	1.095278
10	1	0	-0.778944	-4.359499	-2.271723
11	1	0	-2.249854	-3.580741	-2.814409
12	1	0	-2.025632	-3.942908	-1.100225
13	1	0	-0.084981	-2.658081	-3.764575
14	1	0	0.298979	-1.064177	-3.146065
15	1	0	-1.360467	-1.443212	-3.713399
16	6	0	0.487902	-2.583333	-0.922325
17	6	0	1.076828	-1.324180	-0.383374
18	6	0	0.072191	-3.418441	0.300417
19	6	0	1.513839	-3.364305	-1.764925
20	7	0	1.766976	-0.424736	-1.040881
21	8	0	2.030647	-0.475252	-2.333243
22	8	0	2.157450	0.685357	-0.377824
23	1	0	0.988459	-1.152122	0.669135
24	1	0	0.926417	-3.460260	0.969145
25	1	0	-0.191161	-4.436979	0.038591
26	1	0	-0.744902	-2.967566	0.858023
27	1	0	2.350259	-3.582607	-1.105361
28	1	0	1.904859	-2.775635	-2.582681
29	1	0	1.136298	-4.315621	-2.128899
30	6	0	4.630142	-0.133647	0.524904
31	7	0	4.265732	-0.870476	1.520220
32	6	0	5.073653	-0.491469	-0.859056
33	1	0	4.630538	0.924334	0.746047
34	1	0	5.237557	-1.549702	-1.001631

35	1	0	4.306668	-0.155660	-1.556328
36	1	0	5.980769	0.067892	-1.082597
37	6	0	-2.768938	1.244982	-1.444903
38	6	0	-1.571270	0.255187	-1.339438
39	6	0	-4.011785	0.725905	-2.153147
40	6	0	-1.923670	-1.269423	-1.163520
41	6	0	-4.414229	-0.579672	-1.479551
42	6	0	-3.325856	-1.626446	-1.723913
43	1	0	-3.052612	1.521887	-0.436344
44	1	0	-2.381431	2.140622	-1.926400
45	1	0	-1.008573	0.357127	-2.260528
46	1	0	-4.803391	1.468624	-2.078363
47	1	0	-3.834162	0.557866	-3.217929
48	1	0	-1.901281	-1.501857	-0.107870
49	1	0	-5.350005	-0.964647	-1.881489
50	1	0	-4.558501	-0.414703	-0.413778
51	1	0	-3.652805	-2.567414	-1.296088
52	1	0	-3.271709	-1.763634	-2.803903
53	6	0	0.512448	1.417149	3.046819
54	6	0	1.766144	1.096633	3.579880
55	6	0	-0.446185	2.024269	3.866410
56	6	0	2.050337	1.399765	4.910632
57	1	0	2.506130	0.613614	2.959679
58	6	0	-0.142796	2.295888	5.196100
59	1	0	-1.405956	2.285572	3.464656
60	6	0	1.103199	1.991888	5.738495
61	1	0	1.333126	2.227794	6.761535
62	6	0	-1.186681	2.907898	6.068602
63	6	0	3.389270	1.045126	5.461777
64	9	0	-2.044096	3.738734	5.373179
65	9	0	-1.995060	1.961416	6.687767
66	9	0	3.665285	1.688797	6.651482
67	9	0	3.515453	-0.317532	5.735092
68	9	0	4.424376	1.345242	4.596763
69	8	0	4.411768	-3.199466	0.295053
70	16	0	4.077531	-2.518515	1.559627
71	8	0	2.732167	-2.745062	2.100216
72	6	0	5.273715	-2.984625	2.764429
73	6	0	6.406038	-3.693765	2.360575
74	6	0	5.060141	-2.647475	4.102626
75	6	0	7.347893	-4.066882	3.320374
76	1	0	6.534647	-3.954624	1.324689
77	6	0	6.009542	-3.021498	5.052075
78	1	0	4.177610	-2.109802	4.396769

79	6	0	7.151527	-3.728589	4.662058
80	1	0	8.224265	-4.617588	3.023501
81	1	0	5.857941	-2.760632	6.085286
82	9	0	-0.642616	3.662163	7.092998
83	1	0	7.882073	-4.016124	5.399971

Table 12. Atom coordinates and two energies of **5-s-TS1** (E= -3095.9065 a.u., G= -3096.0314 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.195978	0.001643	0.348953
2	6	0	-0.252415	0.303533	1.609344
3	7	0	0.745503	0.261863	2.547759
4	16	0	-1.871417	0.602698	1.966131
5	7	0	-1.378460	-2.438666	-1.628998
6	6	0	-2.506669	-3.411564	-1.378422
7	6	0	-1.325709	-2.169751	-3.110670
8	1	0	1.190397	-0.135601	0.234780
9	1	0	1.578422	-0.291297	2.334155
10	1	0	-2.367039	-4.290744	-1.987043
11	1	0	-3.449873	-2.961918	-1.642943
12	1	0	-2.528078	-3.687130	-0.333104
13	1	0	-0.956807	-3.045139	-3.625198
14	1	0	-0.665531	-1.340242	-3.321540
15	1	0	-2.314312	-1.935907	-3.479224
16	6	0	0.062343	-3.232081	-1.178341
17	6	0	1.237038	-2.499755	-1.780813
18	6	0	0.120452	-3.212617	0.348668
19	6	0	-0.043847	-4.704813	-1.616261
20	7	0	1.552694	-2.622267	-3.148892
21	8	0	1.303343	-3.686255	-3.813280
22	8	0	2.213048	-1.656786	-3.667148
23	1	0	1.338901	-1.475078	-1.500532
24	1	0	0.913667	-3.875924	0.674856
25	1	0	-0.800176	-3.587660	0.786041
26	1	0	0.325281	-2.238167	0.759535
27	1	0	0.951876	-5.127083	-1.547026
28	1	0	-0.354763	-4.854761	-2.640236
29	1	0	-0.683580	-5.262493	-0.941011
30	6	0	3.175835	-2.695092	-1.033164
31	7	0	3.214199	-1.981438	0.115883
32	6	0	3.557095	-4.153149	-1.173279

33	1	0	3.448503	-2.090055	-1.887909
34	1	0	3.114649	-4.779142	-0.409040
35	1	0	3.294197	-4.515760	-2.161576
36	1	0	4.641627	-4.228023	-1.072293
37	6	0	-1.049666	1.447398	-1.216123
38	6	0	-0.625887	-0.005892	-0.877650
39	6	0	-2.298129	1.544656	-2.084824
40	6	0	-1.744115	-1.106895	-0.817685
41	6	0	-3.434034	0.856494	-1.336585
42	6	0	-3.179167	-0.652681	-1.236922
43	1	0	-1.243881	1.978931	-0.292482
44	1	0	-0.195802	1.925127	-1.692538
45	1	0	0.052991	-0.281529	-1.670669
46	1	0	-2.531886	2.591704	-2.264977
47	1	0	-2.145775	1.084366	-3.064229
48	1	0	-1.793513	-1.451065	0.204275
49	1	0	-4.387308	0.999194	-1.843407
50	1	0	-3.521979	1.291594	-0.346342
51	1	0	-3.885998	-1.080001	-0.531039
52	1	0	-3.429419	-1.053931	-2.213409
53	6	0	0.664946	0.639654	3.904760
54	6	0	-0.057598	1.755213	4.340252
55	6	0	1.409476	-0.098212	4.830970
56	6	0	-0.048944	2.098248	5.688391
57	1	0	-0.612881	2.345999	3.638311
58	6	0	1.410526	0.274272	6.173402
59	1	0	1.978887	-0.946512	4.491378
60	6	0	0.678724	1.367022	6.623960
61	1	0	0.681600	1.644007	7.662621
62	6	0	2.244265	-0.505927	7.133464
63	6	0	-0.863041	3.261206	6.145507
64	9	0	1.876161	-0.296566	8.448644
65	9	0	2.177309	-1.868972	6.912144
66	9	0	-2.158723	2.906282	6.504673
67	9	0	-0.323296	3.879904	7.258544
68	9	0	-0.995950	4.234106	5.172623
69	8	0	2.914071	-3.931478	1.807055
70	16	0	3.403890	-2.552791	1.603429
71	8	0	2.821059	-1.517958	2.488575
72	6	0	5.144421	-2.570588	1.918246
73	6	0	5.776884	-3.784249	2.187929
74	6	0	5.858344	-1.368963	1.902620
75	6	0	7.150964	-3.794782	2.439036
76	1	0	5.199109	-4.691411	2.213833

77	6	0	7.228536	-1.389426	2.153250
78	1	0	5.351554	-0.441066	1.702574
79	6	0	7.875589	-2.601523	2.420075
80	1	0	7.647142	-4.725927	2.654232
81	1	0	7.787313	-0.469090	2.145783
82	9	0	3.594152	-0.179412	7.058937
83	1	0	8.934665	-2.612363	2.617186

Table 13. Atom coordinates and two energies of **5-s-Int2** (E= -3095.9294 a.u., G= -3096.0491 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.516438	0.209896	0.095134
2	6	0	-0.292259	-0.207082	1.382426
3	7	0	0.998906	0.131844	1.759716
4	16	0	-1.393015	-1.084658	2.287366
5	7	0	-1.196183	-2.153287	-2.323029
6	6	0	-1.815664	-3.508439	-2.621805
7	6	0	-1.484090	-1.314242	-3.546420
8	1	0	0.082986	0.962523	-0.205446
9	1	0	1.739317	-0.238872	1.106978
10	1	0	-1.243670	-3.996055	-3.392901
11	1	0	-2.822744	-3.376035	-2.982464
12	1	0	-1.830377	-4.120346	-1.733878
13	1	0	-1.011782	-1.758414	-4.410025
14	1	0	-1.133386	-0.303673	-3.435973
15	1	0	-2.553498	-1.288053	-3.708106
16	6	0	0.452788	-2.458929	-2.130908
17	6	0	1.195371	-1.122682	-1.926066
18	6	0	0.590130	-3.302462	-0.864848
19	6	0	0.958270	-3.275466	-3.332884
20	7	0	1.144743	-0.197841	-3.107031
21	8	0	1.469694	-0.589493	-4.249224
22	8	0	0.813165	0.995958	-2.855813
23	1	0	0.669937	-0.589136	-1.163824
24	1	0	1.624411	-3.615509	-0.752576
25	1	0	-0.004360	-4.207610	-0.926669
26	1	0	0.341306	-2.762251	0.038569
27	1	0	2.036538	-3.197764	-3.340638
28	1	0	0.625495	-2.922463	-4.300308
29	1	0	0.722714	-4.327538	-3.220465
30	6	0	2.711135	-1.027754	-1.398846

31	7	0	2.714413	-1.311416	0.045099
32	6	0	-2.859609	0.820937	-0.171971
33	6	0	-1.692889	-0.025452	-0.760975
34	6	0	-4.261847	0.404419	-0.594404
35	6	0	-1.969372	-1.546305	-1.034052
36	6	0	-4.417809	-1.078568	-0.282922
37	6	0	-3.477884	-1.885770	-1.181464
38	1	0	-2.805897	0.750364	0.907906
39	1	0	-2.656954	1.856314	-0.439024
40	1	0	-1.430951	0.443977	-1.701884
41	1	0	-4.989683	0.999463	-0.047623
42	1	0	-4.438666	0.586253	-1.656790
43	1	0	-1.575612	-2.118901	-0.208254
44	1	0	-5.434285	-1.419796	-0.469567
45	1	0	-4.199607	-1.259687	0.766946
46	1	0	-3.623194	-2.940080	-0.974315
47	1	0	-3.812729	-1.706663	-2.201848
48	6	0	1.431975	0.565896	3.018770
49	6	0	2.810152	0.794470	3.171782
50	6	0	0.580161	0.863348	4.086079
51	6	0	3.306614	1.291759	4.366221
52	1	0	3.476115	0.587932	2.352829
53	6	0	1.107123	1.364565	5.275964
54	1	0	-0.477066	0.705516	3.997351
55	6	0	2.467181	1.583564	5.441495
56	1	0	2.858279	1.974750	6.363650
57	6	0	0.171528	1.630064	6.406771
58	6	0	4.768619	1.539829	4.528066
59	9	0	-1.020487	2.198646	5.988759
60	9	0	-0.189074	0.473016	7.089883
61	9	0	5.050146	2.874823	4.789138
62	9	0	5.308762	0.838065	5.599193
63	9	0	5.506486	1.194698	3.419420
64	8	0	5.174178	-2.009874	0.428111
65	16	0	3.757235	-2.403626	0.589128
66	8	0	3.444889	-3.765630	0.064968
67	6	0	3.444311	-2.432293	2.332510
68	6	0	4.508536	-2.174437	3.196670
69	6	0	2.191195	-2.792655	2.830506
70	6	0	4.310955	-2.265725	4.576313
71	1	0	5.467209	-1.911050	2.786059
72	6	0	1.995140	-2.869981	4.208101
73	1	0	1.378123	-3.006929	2.160454
74	6	0	3.055646	-2.608643	5.082590

75	1	0	5.129320	-2.063277	5.246038
76	1	0	1.023686	-3.127099	4.594699
77	9	0	0.705513	2.478971	7.355426
78	1	0	2.902450	-2.671182	6.147320
79	6	0	3.758380	-1.717942	-2.289717
80	1	0	4.742646	-1.378501	-1.984701
81	1	0	3.756753	-2.796952	-2.185906
82	1	0	3.611695	-1.447592	-3.332172
83	1	0	2.888993	0.044520	-1.505936

Table 14. Atom coordinates and two energies of **5-s-TS2** (E= -3095.8923 a.u., G= -3096.0095 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.361848
3	7	0	1.282911	0.000000	1.860101
4	16	0	-1.403695	-0.007545	2.286921
5	7	0	-2.168706	-2.156522	-1.876527
6	6	0	-3.100076	-3.264807	-1.462436
7	6	0	-2.690344	-1.537597	-3.131242
8	1	0	0.887909	-0.103907	-0.457875
9	1	0	2.013757	0.012617	1.157354
10	1	0	-3.281927	-3.924033	-2.295780
11	1	0	-4.052070	-2.872389	-1.143142
12	1	0	-2.655900	-3.816651	-0.645660
13	1	0	-2.654847	-2.257451	-3.939142
14	1	0	-2.101933	-0.676822	-3.412424
15	1	0	-3.722204	-1.228996	-3.004702
16	6	0	-0.564550	-3.097167	-2.227082
17	6	0	0.330980	-2.166066	-3.113478
18	6	0	0.044149	-3.312099	-0.900492
19	6	0	-1.067416	-4.333945	-2.989604
20	7	0	0.008256	-2.158007	-4.596709
21	8	0	0.196422	-3.188474	-5.283251
22	8	0	-0.385627	-1.068156	-5.082530
23	1	0	0.154823	-1.143118	-2.837265
24	1	0	0.968521	-3.879170	-0.983380
25	1	0	-0.612251	-3.861958	-0.228906
26	1	0	1.547828	-2.158008	-0.930553
27	1	0	-0.184432	-4.792278	-3.424108
28	1	0	-1.755008	-4.162646	-3.815071

29	1	0	-1.485716	-5.053160	-2.299362
30	6	0	1.881727	-2.345087	-3.005838
31	7	0	2.219562	-1.823366	-1.671537
32	6	0	-1.733657	1.517510	-0.845746
33	6	0	-1.165549	0.072093	-0.893122
34	6	0	-3.226580	1.621566	-1.133346
35	6	0	-2.152545	-1.126329	-0.682343
36	6	0	-3.946038	0.753482	-0.107885
37	6	0	-3.628868	-0.731173	-0.333352
38	1	0	-1.560979	1.916990	0.147926
39	1	0	-1.150396	2.122986	-1.536973
40	1	0	-0.743216	-0.030693	-1.882875
41	1	0	-3.539345	2.660583	-1.050066
42	1	0	-3.466719	1.303150	-2.150264
43	1	0	-1.737914	-1.713874	0.123561
44	1	0	-5.026560	0.876991	-0.171807
45	1	0	-3.641726	1.059741	0.887444
46	1	0	-3.922697	-1.291537	0.549797
47	1	0	-4.294819	-1.038492	-1.133287
48	6	0	1.789865	-0.131391	3.160004
49	6	0	3.177611	-0.331860	3.244718
50	6	0	1.049028	-0.072017	4.348002
51	6	0	3.795209	-0.495044	4.478281
52	1	0	3.760534	-0.358150	2.338500
53	6	0	1.697726	-0.233697	5.570652
54	1	0	-0.007916	0.100279	4.308094
55	6	0	3.067729	-0.452466	5.663530
56	1	0	3.548866	-0.576629	6.615996
57	6	0	0.875814	-0.211916	6.817148
58	6	0	5.268808	-0.721881	4.505203
59	9	0	1.626720	0.075311	7.941446
60	9	0	-0.144439	0.717626	6.769627
61	9	0	5.653822	-1.760514	3.661648
62	9	0	5.995457	0.381190	4.082749
63	9	0	5.740730	-1.043134	5.759347
64	8	0	3.249634	-0.269950	-0.099911
65	16	0	3.564556	-0.991265	-1.347234
66	8	0	3.946994	-0.245808	-2.544916
67	6	0	4.889376	-2.097801	-0.967050
68	6	0	5.917369	-2.272085	-1.895057
69	6	0	4.899240	-2.765061	0.260844
70	6	0	6.964904	-3.143124	-1.590949
71	1	0	5.905143	-1.722285	-2.819848
72	6	0	5.951717	-3.628291	0.557371

73	1	0	4.114310	-2.605743	0.979941
74	6	0	6.981489	-3.820858	-0.369544
75	1	0	7.766086	-3.280565	-2.296854
76	1	0	5.974627	-4.132551	1.507712
77	9	0	0.261994	-1.433737	7.073375
78	1	0	7.796556	-4.484685	-0.134660
79	6	0	2.453117	-3.739228	-3.284592
80	1	0	3.537640	-3.691334	-3.229871
81	1	0	2.115493	-4.472749	-2.560915
82	1	0	2.181352	-4.075657	-4.279343
83	1	0	2.302761	-1.655541	-3.735903

Table 15. Atom coordinates and two energies of **5-s-Int3** (E= -3095.9637 a.u., G= -3096.0963 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.293132	0.706645	-0.148975
2	6	0	-1.529912	0.381940	1.143375
3	7	0	-0.338523	0.303146	1.863973
4	16	0	-3.038058	0.067481	1.812151
5	7	0	-1.951544	-1.615737	-1.791510
6	6	0	-2.467657	-2.941402	-1.452661
7	6	0	-1.211241	-1.609351	-3.052271
8	1	0	-0.328394	0.789607	-0.424769
9	1	0	0.501936	0.287599	1.308118
10	1	0	-1.650117	-3.660316	-1.437920
11	1	0	-3.219347	-3.312671	-2.162151
12	1	0	-2.913199	-2.918901	-0.462334
13	1	0	-0.381968	-2.310701	-2.985847
14	1	0	-0.788134	-0.628513	-3.249190
15	1	0	-1.818400	-1.899714	-3.918270
16	6	0	2.451630	-2.562169	0.206067
17	6	0	3.242574	-1.502029	-0.547829
18	6	0	2.927642	-2.982948	1.384048
19	6	0	1.173857	-3.091184	-0.396908
20	7	0	2.270699	-0.511104	-1.158395
21	8	0	2.102935	-0.471626	-2.389061
22	8	0	1.657265	0.243926	-0.354572
23	1	0	3.786272	-0.898801	0.170155
24	1	0	3.816747	-2.568957	1.831714
25	1	0	2.429392	-3.759867	1.940332
26	1	0	5.509353	-3.450736	-0.631307

27	1	0	1.332814	-3.511447	-1.386928
28	1	0	0.411372	-2.317464	-0.492833
29	1	0	0.761514	-3.870522	0.236248
30	6	0	4.266091	-2.007486	-1.606375
31	7	0	5.447753	-2.479310	-0.884327
32	6	0	3.773628	-3.109714	-2.542934
33	1	0	4.568940	-1.155965	-2.209581
34	1	0	3.540931	-4.021515	-1.996736
35	1	0	2.892040	-2.790617	-3.087539
36	1	0	4.556445	-3.334172	-3.261010
37	6	0	-3.255956	1.952927	-1.057420
38	6	0	-2.246765	0.808504	-1.264741
39	6	0	-4.201113	2.096804	-2.255571
40	6	0	-2.935835	-0.531645	-1.602457
41	6	0	-4.916823	0.772151	-2.542712
42	6	0	-3.893496	-0.340765	-2.798231
43	1	0	-3.834329	1.761999	-0.159397
44	1	0	-2.702429	2.876529	-0.893658
45	1	0	-1.626116	1.082322	-2.119193
46	1	0	-4.924810	2.885029	-2.053518
47	1	0	-3.640901	2.403185	-3.142337
48	1	0	-3.531286	-0.806143	-0.737193
49	1	0	-5.575405	0.875385	-3.404356
50	1	0	-5.545447	0.507565	-1.691140
51	1	0	-4.402128	-1.282583	-3.002719
52	1	0	-3.323307	-0.088135	-3.693783
53	6	0	-0.116077	0.158512	3.239737
54	6	0	1.123344	-0.367293	3.628263
55	6	0	-1.014164	0.564681	4.236690
56	6	0	1.451066	-0.488193	4.975042
57	1	0	1.816447	-0.700897	2.874456
58	6	0	-0.665863	0.422001	5.576774
59	1	0	-1.970775	0.963643	3.962262
60	6	0	0.562319	-0.100167	5.972033
61	1	0	0.807615	-0.213824	7.012381
62	6	0	-1.621271	0.901601	6.620205
63	6	0	2.794481	-1.009943	5.351732
64	9	0	-1.494455	2.265644	6.865461
65	9	0	-2.940346	0.701690	6.273514
66	9	0	2.815707	-1.601351	6.595688
67	9	0	3.277245	-1.950203	4.452965
68	9	0	3.770533	-0.012490	5.391550
69	8	0	6.951609	-0.691677	-1.788925
70	16	0	6.816165	-1.599174	-0.652276

71	8	0	7.836730	-2.584777	-0.311813
72	6	0	6.500716	-0.595205	0.769532
73	6	0	6.154911	0.746998	0.601446
74	6	0	6.581343	-1.168955	2.042251
75	6	0	5.853172	1.517447	1.727141
76	1	0	6.142259	1.178381	-0.384507
77	6	0	6.271446	-0.394042	3.158160
78	1	0	6.892773	-2.193348	2.155748
79	6	0	5.899641	0.945987	3.000843
80	1	0	5.587920	2.554106	1.608542
81	1	0	6.316339	-0.826282	4.142370
82	9	0	-1.424943	0.280316	7.839240
83	1	0	5.653621	1.535215	3.867530

Table 16. Atom coordinates and two energies of **5-a-Int1** (E= -3095.9309 a.u., G= -3096.0586 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.514687	0.983211	-0.492900
2	6	0	-0.443632	0.816746	0.860864
3	7	0	0.862007	0.819081	1.280320
4	16	0	-1.796852	0.618321	1.850778
5	7	0	-1.782707	-1.669439	-2.213158
6	6	0	-2.707201	-2.867022	-2.120039
7	6	0	-1.807008	-1.230722	-3.656280
8	1	0	0.374605	1.138425	-0.959053
9	1	0	1.554997	0.846137	0.529676
10	1	0	-2.227484	-3.718802	-2.575026
11	1	0	-3.623351	-2.660562	-2.652286
12	1	0	-2.927907	-3.084293	-1.086509
13	1	0	-1.758475	-2.104042	-4.292623
14	1	0	-0.972536	-0.589864	-3.887584
15	1	0	-2.728613	-0.702469	-3.858853
16	6	0	-0.286730	-2.193536	-1.807680
17	6	0	0.621549	-1.010943	-1.979016
18	6	0	-0.342683	-2.737015	-0.374544
19	6	0	0.168563	-3.324645	-2.754069
20	7	0	1.715185	-0.793560	-1.285521
21	8	0	2.327118	-1.708407	-0.577249
22	8	0	2.181007	0.475071	-1.253203
23	1	0	0.366850	-0.206666	-2.630901
24	1	0	0.636651	-3.111553	-0.113634

25	1	0	-1.032684	-3.569695	-0.287320
26	1	0	-0.590455	-1.984009	0.364288
27	1	0	1.208050	-3.500997	-2.491137
28	1	0	0.148420	-3.043895	-3.802324
29	1	0	-0.357469	-4.264052	-2.610695
30	6	0	3.799888	-2.693210	1.502457
31	7	0	3.207338	-2.795494	2.643346
32	6	0	-2.588508	2.120285	-1.100766
33	6	0	-1.698126	0.870674	-1.348705
34	6	0	-4.028554	2.000916	-1.581011
35	6	0	-2.399858	-0.529934	-1.245941
36	6	0	-4.634514	0.758275	-0.939413
37	6	0	-3.934077	-0.493180	-1.476330
38	1	0	-2.601764	2.312315	-0.035077
39	1	0	-2.079023	2.958532	-1.572107
40	1	0	-1.327101	0.978399	-2.363815
41	1	0	-4.577803	2.895257	-1.294548
42	1	0	-4.089771	1.928649	-2.670243
43	1	0	-2.219417	-0.917147	-0.254208
44	1	0	-5.696521	0.671520	-1.162766
45	1	0	-4.530931	0.818398	0.141519
46	1	0	-4.383073	-1.362909	-1.008932
47	1	0	-4.169663	-0.544143	-2.539000
48	6	0	1.417762	0.768280	2.571848
49	6	0	2.706852	1.292277	2.704647
50	6	0	0.800353	0.190073	3.688365
51	6	0	3.357488	1.262796	3.935473
52	1	0	3.191225	1.730216	1.847488
53	6	0	1.460055	0.199729	4.910614
54	1	0	-0.166527	-0.259470	3.598943
55	6	0	2.740827	0.727588	5.058510
56	1	0	3.236568	0.727493	6.012951
57	6	0	0.803944	-0.389647	6.111985
58	6	0	4.746313	1.792488	4.028178
59	9	0	-0.508296	-0.738087	5.913151
60	9	0	1.450994	-1.538799	6.570628
61	9	0	4.925792	2.955510	3.298004
62	9	0	5.128908	2.072349	5.324384
63	9	0	5.697666	0.900241	3.536120
64	8	0	1.631654	-4.567357	1.566726
65	16	0	1.863381	-3.782175	2.793796
66	8	0	0.777649	-2.938432	3.296486
67	6	0	2.362606	-4.897967	4.063843
68	6	0	2.781924	-6.182951	3.715027

69	6	0	2.320262	-4.480006	5.395111
70	6	0	3.176174	-7.064166	4.722183
71	1	0	2.782580	-6.484197	2.682040
72	6	0	2.717282	-5.369017	6.394010
73	1	0	1.977086	-3.492580	5.644501
74	6	0	3.146886	-6.656521	6.059009
75	1	0	3.498748	-8.059347	4.466732
76	1	0	2.688454	-5.057775	7.424228
77	9	0	0.824575	0.479393	7.197666
78	1	0	3.451658	-7.339317	6.834924
79	6	0	4.947114	-1.769652	1.305495
80	1	0	5.808528	-2.318764	0.925970
81	1	0	4.660960	-1.051971	0.538499
82	1	0	5.213276	-1.256272	2.221094
83	1	0	3.474066	-3.267064	0.643054

Table 17. Atom coordinates and two energies of **5-a-TS1** (E= -3095.8991 a.u., G= -3096.0252 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.369244
3	7	0	1.273708	0.000000	1.879030
4	16	0	-1.401437	-0.073291	2.302092
5	7	0	-2.012524	-2.191258	-1.816232
6	6	0	-2.915645	-3.335438	-1.409208
7	6	0	-2.525957	-1.689514	-3.151026
8	1	0	0.904344	0.087715	-0.439284
9	1	0	2.022196	-0.218790	1.216247
10	1	0	-3.097353	-3.967121	-2.266692
11	1	0	-3.860736	-2.949685	-1.064970
12	1	0	-2.461436	-3.911210	-0.617678
13	1	0	-2.087153	-2.255689	-3.953818
14	1	0	-2.266137	-0.648345	-3.286231
15	1	0	-3.600827	-1.797213	-3.187765
16	6	0	-0.465384	-2.846458	-2.017977
17	6	0	0.489680	-1.859800	-2.652004
18	6	0	0.058701	-3.189833	-0.617454
19	6	0	-0.610269	-4.140208	-2.837924
20	7	0	0.243975	-1.285845	-3.910623
21	8	0	-0.229203	-1.985751	-4.875587
22	8	0	0.606702	-0.076771	-4.087070

23	1	0	0.857996	-1.102543	-1.995739
24	1	0	1.054941	-3.612508	-0.694855
25	1	0	-0.557991	-3.929711	-0.118853
26	1	0	0.142965	-2.319620	0.016512
27	1	0	0.389044	-4.549908	-2.948762
28	1	0	-0.989175	-3.980917	-3.838019
29	1	0	-1.197741	-4.893107	-2.326674
30	6	0	2.445866	-2.607894	-2.983048
31	7	0	3.275641	-1.705725	-2.418633
32	6	0	-1.727918	1.594329	-0.703289
33	6	0	-1.180472	0.146554	-0.875947
34	6	0	-3.206787	1.776952	-1.028044
35	6	0	-2.186699	-1.046323	-0.708633
36	6	0	-3.989304	0.778786	-0.183076
37	6	0	-3.692030	-0.642375	-0.670184
38	1	0	-1.581143	1.892888	0.328393
39	1	0	-1.105016	2.239876	-1.318700
40	1	0	-0.788789	0.110232	-1.884298
41	1	0	-3.498951	2.799380	-0.797784
42	1	0	-3.410730	1.623099	-2.090091
43	1	0	-1.955795	-1.542289	0.222577
44	1	0	-5.063409	0.941479	-0.256331
45	1	0	-3.708595	0.893216	0.858868
46	1	0	-4.232523	-1.341955	-0.039736
47	1	0	-4.124195	-0.704172	-1.663224
48	6	0	1.686583	0.128688	3.217291
49	6	0	1.020567	0.919999	4.156558
50	6	0	2.872666	-0.520686	3.589348
51	6	0	1.528527	1.033205	5.449148
52	1	0	0.122194	1.437115	3.883383
53	6	0	3.365010	-0.380390	4.882275
54	1	0	3.389137	-1.127370	2.863412
55	6	0	2.698012	0.391536	5.832547
56	1	0	3.078317	0.488131	6.833787
57	6	0	4.630783	-1.050545	5.298688
58	6	0	0.761200	1.843042	6.439469
59	9	0	5.671317	-0.147799	5.487247
60	9	0	4.497484	-1.711471	6.512588
61	9	0	1.488204	2.122956	7.578661
62	9	0	0.344200	3.058064	5.921791
63	9	0	-0.395635	1.202684	6.865160
64	8	0	3.350894	-3.143781	-0.291559
65	16	0	3.628957	-1.804489	-0.857205
66	8	0	2.982519	-0.680712	-0.111400

67	6	0	5.363622	-1.497495	-0.803708
68	6	0	5.836973	-0.256566	-0.381528
69	6	0	6.238277	-2.508202	-1.210910
70	6	0	7.213832	-0.026431	-0.356451
71	1	0	5.141727	0.505405	-0.077321
72	6	0	7.610715	-2.269552	-1.182331
73	1	0	5.858597	-3.459585	-1.544280
74	6	0	8.098918	-1.030098	-0.754965
75	1	0	7.589860	0.927630	-0.028484
76	1	0	8.294161	-3.042595	-1.489986
77	9	0	5.080691	-1.975383	4.383748
78	1	0	9.160807	-0.849868	-0.733223
79	6	0	2.561460	-2.741982	-4.475183
80	1	0	1.745397	-3.302521	-4.912152
81	1	0	2.622932	-1.767773	-4.948377
82	1	0	3.495850	-3.268625	-4.668113
83	1	0	2.238231	-3.528669	-2.447960

Table 18. Atom coordinates and two energies of **5-a-Int2** (E= -3095.9322 a.u., G= -3096.0544 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.079279	0.303919	0.500821
2	6	0	-0.614666	0.242276	1.760457
3	7	0	0.335668	0.214006	2.737208
4	16	0	-2.281517	0.123363	2.036652
5	7	0	-1.144596	-1.820835	-2.103321
6	6	0	-2.086411	-3.009729	-2.101321
7	6	0	-1.190802	-1.222906	-3.485857
8	1	0	0.930222	0.185438	0.371718
9	1	0	1.304039	0.054890	2.433215
10	1	0	-1.821825	-3.685583	-2.899040
11	1	0	-3.095310	-2.670031	-2.262491
12	1	0	-2.033494	-3.517887	-1.149640
13	1	0	-0.702156	-1.887702	-4.185163
14	1	0	-0.704859	-0.259942	-3.503638
15	1	0	-2.216373	-1.105881	-3.800780
16	6	0	0.361721	-2.404951	-1.800595
17	6	0	1.452828	-1.360193	-2.238216
18	6	0	0.440134	-2.750902	-0.306646
19	6	0	0.549959	-3.741426	-2.553944
20	7	0	1.700139	-1.332416	-3.739766

21	8	0	2.113178	-2.354144	-4.332899
22	8	0	1.544161	-0.223740	-4.308673
23	1	0	1.146159	-0.350827	-2.048287
24	1	0	1.403138	-3.197400	-0.087136
25	1	0	-0.315531	-3.490882	-0.059194
26	1	0	0.334522	-1.903520	0.344774
27	1	0	1.603679	-3.991685	-2.516337
28	1	0	0.281368	-3.724047	-3.602795
29	1	0	0.013090	-4.539137	-2.056259
30	6	0	2.842933	-1.468014	-1.526960
31	7	0	2.637457	-0.748606	-0.260033
32	6	0	-1.534737	1.860063	-0.748688
33	6	0	-0.861719	0.463226	-0.730706
34	6	0	-2.741473	1.950109	-1.674528
35	6	0	-1.767609	-0.787032	-1.011543
36	6	0	-3.767359	0.930201	-1.194713
37	6	0	-3.254629	-0.502905	-1.396417
38	1	0	-1.859051	2.105981	0.254801
39	1	0	-0.764785	2.577236	-1.024933
40	1	0	-0.131007	0.523720	-1.521639
41	1	0	-3.153578	2.956098	-1.636873
42	1	0	-2.466397	1.764078	-2.716337
43	1	0	-1.767978	-1.383010	-0.112453
44	1	0	-4.706711	1.025068	-1.737476
45	1	0	-3.977127	1.108591	-0.145288
46	1	0	-3.881761	-1.177958	-0.820848
47	1	0	-3.429758	-0.727564	-2.442776
48	6	0	0.196146	0.170837	4.137563
49	6	0	-0.892617	0.691169	4.843880
50	6	0	1.275609	-0.372775	4.852483
51	6	0	-0.897765	0.641459	6.236982
52	1	0	-1.714983	1.132428	4.317514
53	6	0	1.245454	-0.402309	6.241432
54	1	0	2.128566	-0.746293	4.310662
55	6	0	0.157492	0.093905	6.956357
56	1	0	0.146491	0.077220	8.031205
57	6	0	2.381609	-1.020489	6.985120
58	6	0	-2.088613	1.166405	6.965671
59	9	0	2.545737	-0.472833	8.245912
60	9	0	2.207298	-2.385933	7.191371
61	9	0	-1.796130	1.537955	8.264650
62	9	0	-2.646956	2.272677	6.351083
63	9	0	-3.116343	0.233622	7.062569
64	8	0	3.512447	-2.724620	1.099436

65	16	0	3.441334	-1.247460	1.003790
66	8	0	2.841835	-0.537620	2.166558
67	6	0	5.133031	-0.697873	0.963301
68	6	0	5.405129	0.672655	0.924957
69	6	0	6.168034	-1.632491	0.974172
70	6	0	6.727986	1.108457	0.887921
71	1	0	4.595372	1.381903	0.928417
72	6	0	7.493075	-1.189113	0.935435
73	1	0	5.931945	-2.680848	1.024302
74	6	0	7.773724	0.177704	0.891088
75	1	0	6.944279	2.163302	0.862510
76	1	0	8.296863	-1.906026	0.947956
77	9	0	3.588638	-0.888155	6.331695
78	1	0	8.795982	0.517403	0.865359
79	6	0	3.969556	-0.825453	-2.354518
80	1	0	4.881350	-0.853012	-1.767529
81	1	0	4.163182	-1.346732	-3.288213
82	1	0	3.745256	0.217871	-2.561758
83	1	0	3.084833	-2.521503	-1.374535

Table 19. Atom coordinates and two energies of **5-a-TS2** (E= -3095.8905 a.u., G= -3096.0103 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.361385	-1.844083	-1.010052
2	6	0	0.855183	-1.969404	-0.399340
3	7	0	1.603897	-0.817668	-0.530180
4	16	0	1.304527	-3.334421	0.463197
5	1	0	-0.504454	-1.066161	-1.635550
6	1	0	1.062115	0.032697	-0.650474
7	7	0	-3.870135	-2.213429	0.244337
8	6	0	-5.014051	-2.932066	-0.390913
9	6	0	-3.377821	-3.088946	1.356222
10	6	0	-4.559383	-0.584094	0.971361
11	6	0	-3.327017	-0.008122	1.767373
12	6	0	-4.925599	0.272247	-0.156735
13	6	0	-5.702600	-1.105349	1.842926
14	7	0	-3.632395	-0.001819	3.242433
15	8	0	-4.324500	0.936537	3.699700
16	8	0	-3.185964	-0.949070	3.931938
17	6	0	-2.808567	1.410120	1.364271
18	7	0	-2.526661	1.307929	-0.079727

19	1	0	-5.709402	-3.249413	0.374082
20	1	0	-4.651456	-3.814031	-0.906943
21	1	0	-5.523150	-2.289745	-1.093048
22	1	0	-4.180900	-3.254954	2.059713
23	1	0	-2.548933	-2.646259	1.888224
24	1	0	-3.067651	-4.052249	0.963584
25	1	0	-2.484508	-0.678439	1.682308
26	1	0	-5.094353	1.295499	0.179444
27	1	0	-5.803876	-0.068079	-0.697175
28	1	0	-6.114588	-0.242431	2.359975
29	1	0	-5.438623	-1.838191	2.599513
30	1	0	-6.498911	-1.491136	1.219321
31	1	0	-3.455380	0.881936	-0.560644
32	6	0	-1.614452	1.823396	2.228767
33	1	0	-1.250121	2.799748	1.924530
34	1	0	-1.916958	1.904106	3.268070
35	1	0	-0.789865	1.123148	2.145631
36	1	0	-3.609176	2.128566	1.519715
37	6	0	2.945941	-0.582859	-0.200359
38	6	0	3.945182	-1.561232	-0.213549
39	6	0	3.292446	0.741024	0.102436
40	6	0	5.257697	-1.204137	0.086949
41	1	0	3.700339	-2.578207	-0.450153
42	6	0	4.611789	1.071732	0.386817
43	1	0	2.523547	1.494790	0.120533
44	6	0	5.614580	0.105880	0.391031
45	1	0	6.632895	0.363804	0.619514
46	6	0	4.965333	2.495283	0.654454
47	6	0	6.302107	-2.270418	0.114641
48	9	0	5.337896	3.182504	-0.497100
49	9	0	3.912723	3.215209	1.191738
50	9	0	6.027161	2.625566	1.528030
51	9	0	6.090161	-3.247560	-0.839328
52	9	0	7.572967	-1.770325	-0.100835
53	9	0	6.358635	-2.936102	1.332977
54	8	0	-1.445830	1.175367	-2.257887
55	16	0	-1.279162	1.811333	-0.940927
56	8	0	0.010743	1.534254	-0.266949
57	6	0	-1.372395	3.565676	-1.130844
58	6	0	-2.461359	4.107797	-1.820234
59	6	0	-0.368433	4.380280	-0.606965
60	6	0	-2.545420	5.489128	-1.978431
61	1	0	-3.219824	3.463997	-2.232828
62	6	0	-0.461995	5.764296	-0.770178

63	1	0	0.467482	3.940177	-0.092467
64	6	0	-1.547286	6.317558	-1.452305
65	1	0	-3.377703	5.916914	-2.510805
66	1	0	0.309531	6.400688	-0.371835
67	1	0	-4.215326	-1.110223	-2.211000
68	6	0	-3.253245	-1.603563	-2.220961
69	6	0	-2.767192	-1.837038	-0.769382
70	6	0	-3.245423	-2.814991	-3.165372
71	1	0	-2.576339	-0.855809	-2.632509
72	6	0	-1.496199	-2.738322	-0.743814
73	1	0	-2.439029	-0.875372	-0.413177
74	6	0	-1.894751	-3.536034	-3.136107
75	1	0	-4.035770	-3.523650	-2.919602
76	1	0	-3.458964	-2.458887	-4.172096
77	6	0	-1.538840	-3.936463	-1.704186
78	1	0	-1.307044	-3.127230	0.246157
79	1	0	-1.918877	-4.417980	-3.773477
80	1	0	-1.118841	-2.882555	-3.536225
81	1	0	-0.573573	-4.432109	-1.660158
82	1	0	-2.277252	-4.653886	-1.335335
83	1	0	-1.615011	7.385217	-1.577996

Table 20. Atom coordinates and two energies of **5-a-Int3** (E= -3095.9633 a.u., G= -3096.0982 a.u.)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.417857	0.768664	-0.812859
2	6	0	-1.148062	0.857248	0.511511
3	7	0	0.217457	1.038953	0.730916
4	16	0	-2.269100	0.797962	1.757478
5	7	0	-2.594548	-1.850618	-1.386169
6	6	0	-2.892703	-2.992472	-0.522271
7	6	0	-2.422867	-2.238952	-2.785072
8	1	0	-0.626253	0.683791	-1.428867
9	1	0	0.769703	1.236142	-0.088699
10	1	0	-2.117161	-3.749262	-0.630671
11	1	0	-3.853344	-3.473967	-0.748837
12	1	0	-2.907724	-2.673005	0.515803
13	1	0	-1.594931	-2.938878	-2.868098
14	1	0	-2.179736	-1.375169	-3.398031
15	1	0	-3.307717	-2.721343	-3.217754
16	6	0	2.091853	-2.673499	-1.852205

17	6	0	2.552413	-1.395427	-1.167585
18	6	0	0.873527	-3.145211	-1.557796
19	6	0	3.032808	-3.349441	-2.815413
20	7	0	2.455913	-0.240222	-2.146296
21	8	0	3.233993	-0.203185	-3.114792
22	8	0	1.568258	0.631529	-1.928948
23	1	0	1.859151	-1.125511	-0.380148
24	1	0	0.194781	-2.634437	-0.891810
25	1	0	0.516587	-4.060565	-2.002267
26	1	0	3.193318	-3.195196	0.348442
27	1	0	3.934846	-3.699215	-2.316179
28	1	0	3.342796	-2.671329	-3.607039
29	1	0	2.551858	-4.209177	-3.271007
30	6	0	3.989364	-1.443250	-0.604445
31	7	0	3.972370	-2.556365	0.359045
32	6	0	-3.607838	1.882126	-1.239821
33	6	0	-2.726737	0.640770	-1.476348
34	6	0	-4.950952	1.773050	-1.970102
35	6	0	-3.455596	-0.677454	-1.136420
36	6	0	-5.684295	0.489840	-1.565389
37	6	0	-4.813578	-0.735000	-1.868309
38	1	0	-3.783650	1.998766	-0.175235
39	1	0	-3.060991	2.762686	-1.574235
40	1	0	-2.485193	0.619683	-2.539825
41	1	0	-5.557971	2.647932	-1.742549
42	1	0	-4.792818	1.772062	-3.051291
43	1	0	-3.651069	-0.661369	-0.068893
44	1	0	-6.632697	0.411422	-2.095466
45	1	0	-5.916640	0.524746	-0.500012
46	1	0	-5.333593	-1.649034	-1.582839
47	1	0	-4.653263	-0.786576	-2.946540
48	6	0	0.909771	1.141661	1.950367
49	6	0	1.983218	2.035856	2.014599
50	6	0	0.630444	0.338581	3.062580
51	6	0	2.768897	2.112530	3.161730
52	1	0	2.192038	2.677239	1.174392
53	6	0	1.418753	0.447262	4.205084
54	1	0	-0.190106	-0.352141	3.027379
55	6	0	2.495079	1.326675	4.274784
56	1	0	3.097465	1.394076	5.161658
57	6	0	1.097429	-0.432492	5.367543
58	6	0	3.949883	3.022165	3.164373
59	9	0	-0.145087	-0.175103	5.915091
60	9	0	1.079565	-1.778483	5.017559

61	9	0	3.704850	4.215898	2.512524
62	9	0	4.384669	3.333747	4.434222
63	9	0	5.047506	2.461030	2.510739
64	8	0	6.468278	-2.714493	0.340129
65	16	0	5.307728	-3.144191	1.118376
66	8	0	5.008279	-4.555938	1.347296
67	6	0	5.396235	-2.345578	2.693290
68	6	0	6.351465	-1.353054	2.912868
69	6	0	4.513028	-2.738829	3.702920
70	6	0	6.409400	-0.729867	4.160795
71	1	0	7.043013	-1.088898	2.132051
72	6	0	4.575592	-2.109322	4.944250
73	1	0	3.804492	-3.530188	3.529254
74	6	0	5.522219	-1.104362	5.172404
75	1	0	7.143153	0.037091	4.339848
76	1	0	3.899231	-2.404101	5.727508
77	9	0	2.012171	-0.313543	6.395799
78	1	0	5.571268	-0.624462	6.135681
79	6	0	4.393624	-0.119253	0.044556
80	1	0	4.365921	0.694032	-0.677087
81	1	0	3.743038	0.120140	0.880562
82	1	0	5.411829	-0.176673	0.410604
83	1	0	4.680873	-1.665456	-1.412907
