

Supporting Information

Understanding the Reactivity and Activation Barrier Origins in the Cycloaddition of Triplet Pnictinidenes with Phenylacetylene

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Table SA. The total number of atoms and basis functions (M06-2X-D3/def2-SVP) involved in these molecular systems is summarized in the table. As shown therein, for instance, the **[Bi-T/S]** system comprises 188 atoms and 1723 basis functions, representing a computationally demanding system. Even at the def2-SVP level, the calculations are already computationally intensive, and the use of larger basis sets, such as def2-TZVP, would result in a prohibitive increase in computational cost.

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PhC≡CH pathway (188 atom numbers):

N: 1705 basis functions

P: 1709 basis functions

As: 1717 basis functions

Sb: 1723 basis functions

Bi: 1723 basis functions

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Table SB. The computed energies for the intersystem crossing points, denoted as **[G15-T/S-]**.

Crossing Points	Triplet state (Hartree)	Singlet state (Hartree)
[N-T/S]	-3313.9101064200	-3313.9101097400
[P-T/S]	-3600.4496057800	-3600.4496070600
[As-T/S]	-5494.8427430300	-5494.8427412300
[Sb-T/S]	-3499.3968079600	-3499.3968222600
[Bi-T/S]	-3473.7131809100	-3473.7131739400

Figure S1. Optimized structures at the M06-2X-D3/def2-SVP level (bond lengths in Å) for the triplet ground-state pnictinidene **[G15-Rea]³**.

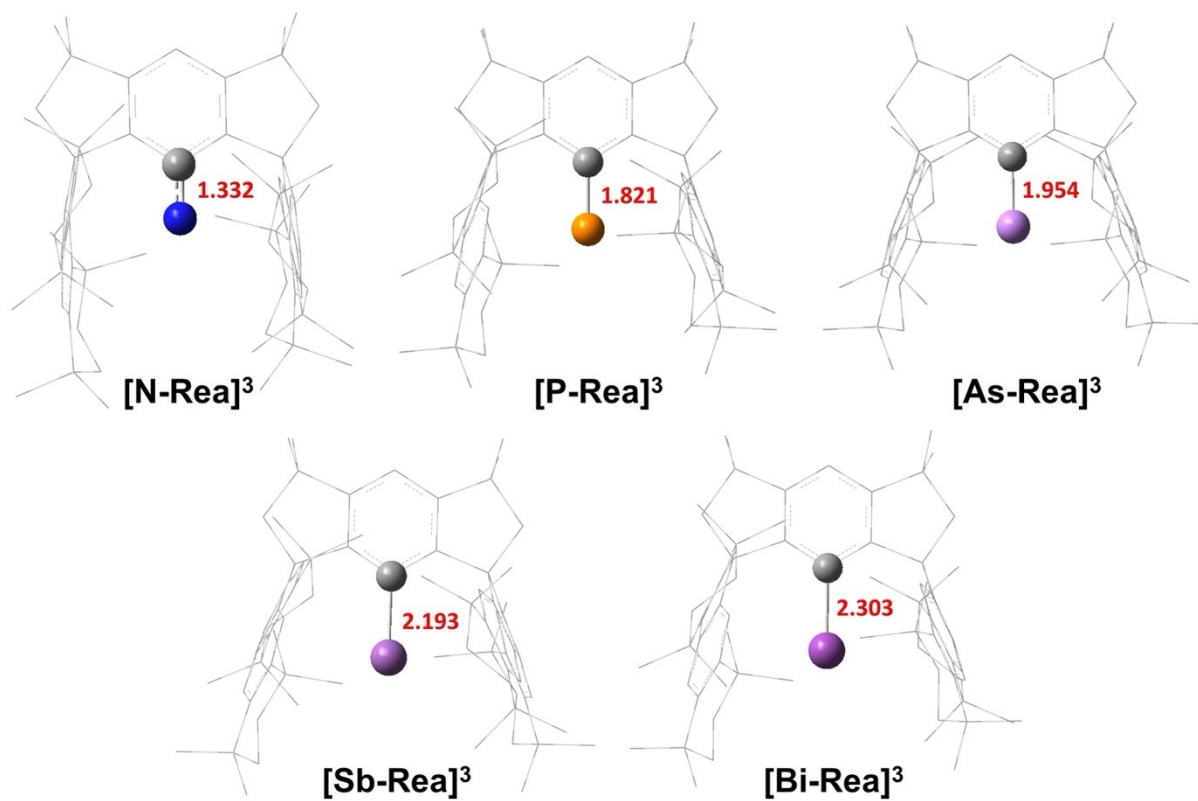
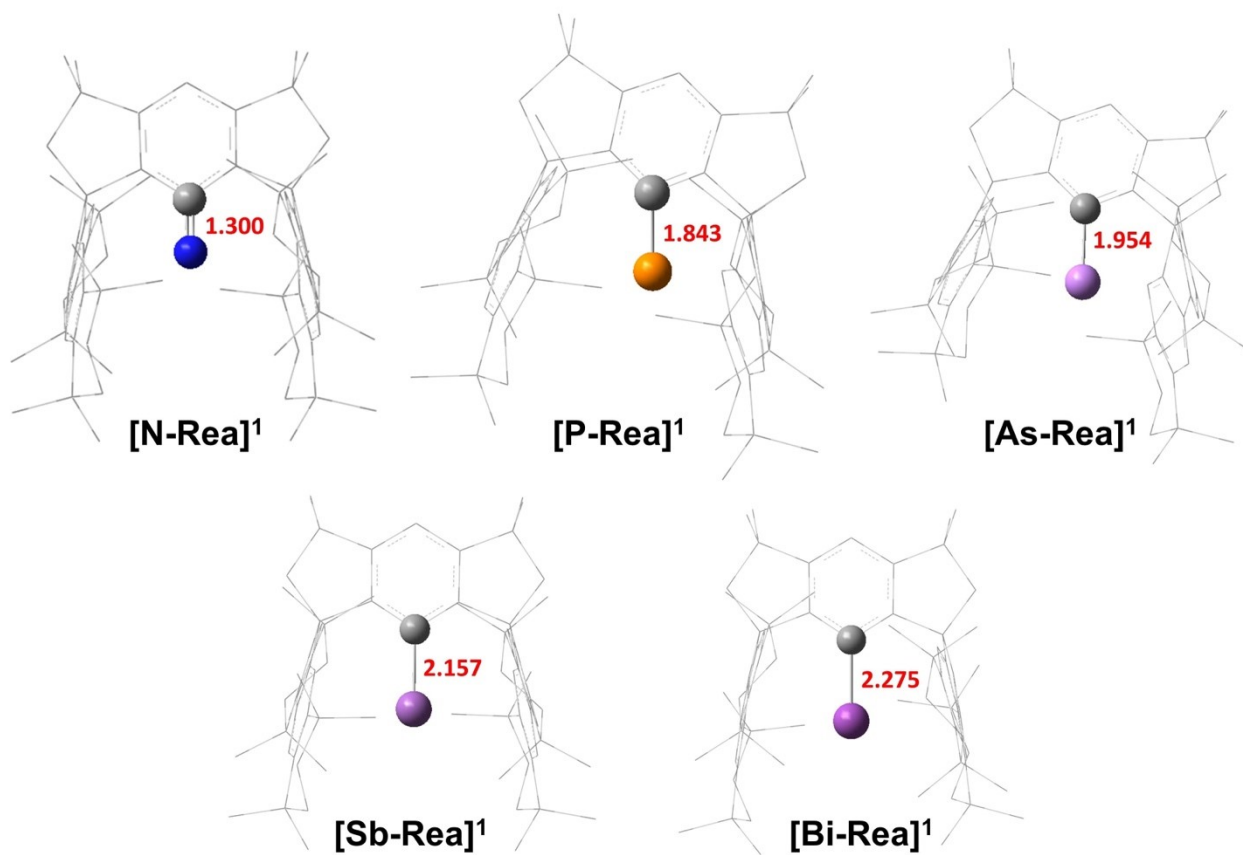


Figure S2. Optimized structures at the M06-2X-D3/def2-SVP level (bond lengths in Å) for the singlet pnictinidene [G15-Rea]¹.



(All were calculated at the M06-2X-D3/def2-SVP level of theory)

Table S1

[N-Rea]³

E : -2848.75711678 Hartree

G : -2847.423458 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	0.000002	-0.000017	0.941781
6	-0.000469	-0.000237	2.274093
6	1.200503	-0.178854	3.028902
6	-1.201978	0.178129	3.028106
6	2.585937	-0.379712	2.445658
6	1.199435	-0.128524	4.413344
6	-2.586993	0.379185	2.443937
6	-1.201899	0.127369	4.412534
6	3.496819	-0.169908	3.691280
6	2.779645	0.579336	1.279116
6	2.745196	-1.728099	1.740491
6	2.610644	-0.205448	4.975950
6	-0.001485	-0.000682	5.127699
6	-3.498765	0.168921	3.688829

6	-2.745735	1.727839	1.739164
6	-2.779887	-0.579422	1.276902
6	-2.613515	0.204061	4.974148
1	4.298012	-0.921576	3.725562
1	3.980397	0.814445	3.607245
6	2.947430	-0.110425	0.072806
6	2.571636	1.943954	1.274958
6	2.977979	-1.550825	0.367065
6	2.691431	-3.006016	2.264109
6	2.900570	1.008928	5.866548
6	2.813177	-1.486184	5.795369
1	-0.001867	-0.000845	6.221465
1	-4.300003	0.920555	3.722793
1	-3.982250	-0.815417	3.604108
6	-2.977563	1.551082	0.365508
6	-2.692282	3.005560	2.263292
6	-2.946831	0.110790	0.070730
6	-2.571936	-1.944046	1.272390
6	-2.904020	-1.010635	5.864123
6	-2.816702	1.484506	5.793857
6	2.903091	0.581335	-1.129237
6	2.467928	2.651465	0.066764
1	2.385026	2.457763	2.221859
6	3.160683	-2.655124	-0.452327

6	2.891184	-4.138179	1.451161
1	2.494954	-3.142018	3.327749
1	2.722675	1.946212	5.318799
1	2.259248	1.007942	6.761112
1	3.949118	0.996978	6.201743
1	2.133491	-1.504435	6.660894
1	3.845835	-1.543809	6.171696
1	2.614877	-2.385673	5.196889
6	-3.159661	2.655693	-0.453599
6	-2.891459	4.138031	1.450631
1	-2.496509	3.141153	3.327115
6	-2.901709	-0.580540	-1.131533
6	-2.467458	-2.651130	0.064009
1	-2.386018	-2.458215	2.219232
1	-2.725655	-1.947724	5.316190
1	-2.263355	-1.009906	6.759158
1	-3.952816	-0.998867	6.198547
1	-2.137608	1.502522	6.659852
1	-3.849622	1.541922	6.169499
1	-2.618081	2.384212	5.195810
6	2.627213	1.958132	-1.154436
1	3.011911	0.033353	-2.066507
6	2.014931	4.110653	0.145022
6	3.142182	-3.959089	0.073277

1	3.332020	-2.504532	-1.520107
6	2.894673	-5.517707	2.117942
6	-3.141510	3.959462	0.072505
1	-3.330241	2.505500	-1.521557
6	-2.895399	5.517307	2.117933
6	-2.625896	-1.957343	-1.157045
1	-3.009883	-0.032221	-2.068681
6	-2.014647	-4.110389	0.142043
6	2.495110	2.651289	-2.515508
6	2.199764	4.812936	-1.206858
6	0.527500	4.104638	0.544755
6	2.808501	4.897078	1.197338
6	3.369730	-5.125959	-0.897474
6	2.697812	-6.610240	1.057403
6	1.769818	-5.657041	3.154279
6	4.240424	-5.707123	2.841391
6	-3.368325	5.126709	-0.897964
6	-2.697737	6.610238	1.057956
6	-1.771308	5.656223	3.155157
6	-4.241684	5.706483	2.840448
6	-2.492958	-2.650024	-2.518276
6	-2.198674	-4.812169	-1.210206
6	-0.527470	-4.104673	0.542724
6	-2.808961	-4.897120	1.193570

6	1.713599	3.966441	-2.369032
6	1.727845	1.774309	-3.516746
6	3.902563	2.923200	-3.072741
1	1.664708	5.776593	-1.181086
1	3.266855	5.055393	-1.343099
1	0.145671	5.136451	0.618418
1	0.386544	3.616378	1.521631
1	-0.095111	3.551034	-0.174316
1	2.519889	5.958993	1.157649
1	3.890003	4.827162	1.008262
1	2.613862	4.543097	2.219286
6	4.592168	-4.863329	-1.790404
6	3.625373	-6.433925	-0.131772
6	2.131355	-5.281814	-1.797265
1	1.648233	-6.589771	0.717758
1	2.854244	-7.595024	1.526360
1	1.734942	-6.695312	3.518364
1	0.792539	-5.412204	2.715063
1	1.925022	-5.011024	4.030016
1	5.092034	-5.618636	2.152768
1	4.365714	-4.938108	3.618285
1	4.281117	-6.695746	3.325611
6	-4.590146	4.864482	-1.791857
6	-3.624451	6.434399	-0.131950

6	-2.129312	5.282833	-1.796826
1	-1.647912	6.589888	0.719065
1	-2.854495	7.594842	1.527180
1	-1.927179	5.009884	4.030539
1	-0.793712	5.411524	2.716572
1	-1.736672	6.694356	3.519661
1	-4.367606	4.937143	3.616917
1	-4.282689	6.694903	3.325057
1	-5.092777	5.618341	2.151139
6	-1.711668	-3.965303	-2.371759
6	-1.724961	-1.772753	-3.518694
6	-3.900075	-2.921597	-3.076530
1	-1.663731	-5.775888	-1.184436
1	-3.265700	-5.054471	-1.347231
1	-0.145781	-5.136552	0.616196
1	-0.387094	-3.616833	1.519894
1	0.095647	-3.550824	-0.175720
1	-2.614914	-4.543546	2.215771
1	-3.890339	-4.827022	1.003852
1	-2.520434	-5.959050	1.153658
1	0.645551	3.730320	-2.229934
1	1.787914	4.528239	-3.314239
1	0.772888	1.436040	-3.087457
1	1.514050	2.357760	-4.425548

1	2.300159	0.888763	-3.826029
1	4.459831	1.980838	-3.180694
1	3.838480	3.402444	-4.062504
1	4.484525	3.574866	-2.405900
1	5.478549	-4.628684	-1.182699
1	4.810960	-5.761466	-2.388605
1	4.427238	-4.033368	-2.491305
1	4.671687	-6.449869	0.213861
1	3.521522	-7.277657	-0.832689
1	2.301305	-6.071630	-2.545623
1	1.236023	-5.541353	-1.214751
1	1.917938	-4.343539	-2.331406
1	-5.476969	4.629654	-1.184867
1	-4.808469	5.762858	-2.389871
1	-4.424764	4.034779	-2.492955
1	-4.671011	6.450257	0.212944
1	-3.520068	7.278390	-0.832475
1	-2.298669	6.072969	-2.544982
1	-1.234360	5.542042	-1.213582
1	-1.915608	4.344759	-2.331205
1	-0.643686	-3.729335	-2.231879
1	-1.785422	-4.526756	-3.317214
1	-0.770235	-1.434757	-3.088677
1	-2.296982	-0.887024	-3.827998

1	-1.510660	-2.355880	-4.427584
1	-4.457168	-1.979136	-3.184525
1	-3.835391	-3.400507	-4.066415
1	-4.482550	-3.573426	-2.410298

Table S2

[P-Rea]³

E : -3135.34880332 Hartree

G : -3134.017566 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
15	0.000140	0.000135	0.428315
6	-0.000394	-0.000068	2.249421
6	1.192458	-0.090198	2.998324
6	-1.193667	0.089916	2.997669
6	2.602515	-0.232509	2.446473
6	1.196039	-0.063569	4.394503
6	-2.603425	0.232306	2.445055
6	-1.198032	0.063041	4.393842
6	3.488464	0.043592	3.700602
6	2.890921	0.709407	1.289981

6	2.852215	-1.586043	1.782153
6	2.602596	-0.098445	4.969860
6	-0.001197	-0.000325	5.108842
6	-3.490060	-0.044042	3.698634
6	-2.852752	1.585955	1.780828
6	-2.891179	-0.709413	1.288240
6	-2.604912	0.097832	4.968411
1	4.365903	-0.618151	3.725648
1	3.861071	1.076393	3.633632
6	3.358014	0.017799	0.165494
6	2.602263	2.058139	1.209209
6	3.357280	-1.419899	0.481132
6	2.613542	-2.859041	2.264725
6	2.829913	1.078400	5.926076
6	2.868914	-1.409629	5.721313
1	-0.001504	-0.000417	6.202949
1	-4.367554	0.617642	3.723298
1	-3.862566	-1.076855	3.631284
6	-3.357080	1.420031	0.479491
6	-2.614333	2.858871	2.263737
6	-3.357638	-0.017612	0.163606
6	-2.602511	-2.058137	1.207406
6	-2.832770	-1.079144	5.924338
6	-2.871666	1.408910	5.719889

6	3.561940	0.701493	-1.025642
6	2.734685	2.749187	-0.005800
1	2.174542	2.561252	2.080234
6	3.658267	-2.531864	-0.290850
6	2.916924	-3.999724	1.496680
1	2.162137	-2.981241	3.250207
1	2.593948	2.033192	5.433436
1	2.197197	0.989559	6.822373
1	3.879902	1.107777	6.255893
1	2.154329	-1.535452	6.548899
1	3.885431	-1.408490	6.143702
1	2.779303	-2.280919	5.059048
6	-3.657622	2.532121	-0.292483
6	-2.917285	3.999681	1.495707
1	-2.163481	2.980918	3.249492
6	-3.560926	-0.701103	-1.027751
6	-2.734269	-2.748983	-0.007793
1	-2.175272	-2.561402	2.078579
1	-2.596523	-2.033869	5.431702
1	-2.200567	-0.990424	6.821009
1	-3.882948	-1.108569	6.253550
1	-2.157539	1.534634	6.547885
1	-3.888415	1.407699	6.141718
1	-2.781704	2.280292	5.057792

6	3.239046	2.064729	-1.136050
1	3.922998	0.158433	-1.900372
6	2.165703	4.168154	-0.081453
6	3.469273	-3.833036	0.208108
1	4.037468	-2.392274	-1.305268
6	2.682154	-5.377222	2.125913
6	-3.468894	3.833211	0.206793
1	-4.036258	2.392702	-1.307135
6	-2.682840	5.377063	2.125310
6	-3.237999	-2.064330	-1.138204
1	-3.921479	-0.157891	-1.902596
6	-2.165222	-4.167927	-0.083377
6	3.472251	2.765479	-2.479762
6	2.694345	4.897274	-1.324181
6	0.630472	4.043454	-0.147278
6	2.538962	5.002975	1.150947
6	3.829331	-5.010506	-0.706686
6	2.679183	-6.459295	1.036805
6	1.334422	-5.447254	2.858939
6	3.802586	-5.645000	3.146881
6	-3.828390	5.010836	-0.708019
6	-2.679307	6.459350	1.036407
6	-1.335490	5.446932	2.859056
6	-3.803806	5.644654	3.145743

6	-3.470480	-2.764863	-2.482154
6	-2.693154	-4.896839	-1.326527
6	-0.629964	-4.043182	-0.148334
6	-2.539142	-5.002987	1.148667
6	2.621442	4.041379	-2.576408
6	3.090943	1.866423	-3.664691
6	4.967100	3.114568	-2.588718
1	2.119183	5.827361	-1.460883
1	3.738060	5.202623	-1.141633
1	0.167463	5.044269	-0.165934
1	0.241703	3.498653	0.728175
1	0.300381	3.486932	-1.036618
1	2.199335	6.040643	1.007808
1	3.628362	5.015282	1.304290
1	2.065736	4.630008	2.069870
6	5.219088	-4.814943	-1.331134
6	3.855517	-6.326292	0.086338
6	2.789456	-5.100591	-1.836728
1	1.734380	-6.388513	0.471541
1	2.680232	-7.450163	1.518734
1	1.156559	-6.479213	3.198641
1	0.508720	-5.157298	2.193833
1	1.305019	-4.801906	3.748136
1	4.796801	-5.617121	2.679618

1	3.789355	-4.879109	3.936907
1	3.664253	-6.630097	3.619871
6	-5.217751	4.815381	-1.333384
6	-3.855090	6.326465	0.085240
6	-2.787806	5.101134	-1.837385
1	-1.734175	6.388763	0.471666
1	-2.680697	7.450119	1.518539
1	-1.306568	4.801402	3.748138
1	-0.509449	5.157087	2.194324
1	-1.157787	6.478820	3.199055
1	-3.791014	4.878620	3.935637
1	-3.665722	6.629661	3.618992
1	-4.797770	5.616872	2.677939
6	-2.619575	-4.040719	-2.578557
6	-3.088589	-1.865604	-3.666742
6	-4.965261	-3.113976	-2.591937
1	-2.117892	-5.826886	-1.463076
1	-3.736962	-5.202247	-1.144612
1	-0.166928	-5.043986	-0.166866
1	-0.241700	-3.498486	0.727411
1	-0.299387	-3.486532	-1.037414
1	-2.066402	-4.630195	2.067911
1	-3.628623	-5.015324	1.301429
1	-2.199435	-6.040625	1.005511

1	1.574241	3.756218	-2.769437
1	2.951655	4.618004	-3.455494
1	2.070247	1.473185	-3.547291
1	3.131247	2.452106	-4.595863
1	3.777151	1.016923	-3.785926
1	5.578700	2.202578	-2.523215
1	5.177691	3.604517	-3.552535
1	5.287432	3.784476	-1.778395
1	5.976523	-4.635008	-0.554014
1	5.503825	-5.721398	-1.887549
1	5.245462	-3.973506	-2.037267
1	4.797214	-6.383638	0.656366
1	3.875634	-7.166655	-0.625944
1	3.050589	-5.912731	-2.533154
1	1.781228	-5.288846	-1.442548
1	2.749292	-4.159397	-2.404695
1	-5.975687	4.635322	-0.556781
1	-5.502124	5.721927	-1.889834
1	-5.243677	3.974064	-2.039677
1	-4.797123	6.383641	0.654731
1	-3.874842	7.166957	-0.626899
1	-3.048506	5.913383	-2.533847
1	-1.779828	5.289326	-1.442546
1	-2.747279	4.160028	-2.405476

1	-1.572274	-3.755492	-2.770949
1	-2.949281	-4.617201	-3.457927
1	-2.067974	-1.472339	-3.548745
1	-3.774774	-1.016118	-3.788206
1	-3.128378	-2.451148	-4.598024
1	-5.576924	-2.202013	-2.526639
1	-5.175336	-3.603810	-3.555925
1	-5.286002	-3.783995	-1.781867

Table S3

[As-Rea]³

E : -5029.75985200 Hartree

G : -5028.429603 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
33	-0.000088	0.000209	0.288623
6	0.000045	0.000139	2.243041
6	1.193330	-0.070193	2.986815
6	-1.193146	0.070445	2.986972
6	2.608608	-0.199432	2.441334
6	1.196748	-0.048834	4.385081

6	-2.608506	0.199605	2.441681
6	-1.196374	0.049117	4.385240
6	3.488121	0.083322	3.698986
6	2.916960	0.743302	1.291051
6	2.870962	-1.551935	1.781098
6	2.601649	-0.077123	4.963973
6	0.000235	0.000155	5.099581
6	-3.487838	-0.083110	3.699470
6	-2.871012	1.552048	1.781390
6	-2.916997	-0.743223	1.291506
6	-2.601196	0.077464	4.964319
1	4.375666	-0.564944	3.722312
1	3.844703	1.122088	3.637580
6	3.422355	0.053710	0.181485
6	2.636668	2.093483	1.204665
6	3.409283	-1.384868	0.493770
6	2.608738	-2.824579	2.252569
6	2.818129	1.091541	5.932525
6	2.876958	-1.394039	5.702299
1	0.000309	0.000172	6.193708
1	-4.375401	0.565129	3.722882
1	-3.844396	-1.121891	3.638184
6	-3.409543	1.384875	0.494166
6	-2.608680	2.824730	2.252706

6	-3.422628	-0.053728	0.181986
6	-2.636585	-2.093381	1.205138
6	-2.817560	-1.091069	5.933048
6	-2.876386	1.394490	5.702497
6	3.671125	0.740488	-0.999122
6	2.820003	2.789492	-0.001364
1	2.182760	2.596032	2.062696
6	3.715217	-2.496347	-0.277196
6	2.918797	-3.964735	1.486744
1	2.131065	-2.945346	3.225852
1	2.574116	2.049333	5.449728
1	2.185604	0.987747	6.827350
1	3.867568	1.126581	6.263603
1	2.159072	-1.536509	6.524294
1	3.891163	-1.387202	6.130249
1	2.800536	-2.258312	5.029275
6	-3.715554	2.496290	-0.276862
6	-2.918808	3.964823	1.486816
1	-2.130862	2.945568	3.225910
6	-3.671534	-0.740589	-0.998546
6	-2.820046	-2.789461	-0.000828
1	-2.182476	-2.595841	2.063117
1	-2.573636	-2.048928	5.450338
1	-2.184908	-0.987173	6.827770

1	-3.866952	-1.126046	6.264280
1	-2.158388	1.537071	6.524375
1	-3.890536	1.387736	6.130581
1	-2.800037	2.258660	5.029330
6	3.360810	2.106376	-1.115411
1	4.062421	0.199301	-1.861992
6	2.274771	4.217220	-0.089400
6	3.498483	-3.797478	0.210038
1	4.115001	-2.356006	-1.283504
6	2.663733	-5.342654	2.107510
6	-3.498675	3.797458	0.210204
1	-4.115513	2.355866	-1.283089
6	-2.663628	5.342792	2.107428
6	-3.361131	-2.106457	-1.114811
1	-4.063025	-0.199483	-1.861377
6	-2.274627	-4.217117	-0.088871
6	3.650744	2.810270	-2.446517
6	2.863751	4.945842	-1.304981
6	0.741659	4.118190	-0.216609
6	2.612298	5.037897	1.162740
6	3.847326	-4.974921	-0.708694
6	2.668766	-6.422580	1.016324
6	1.305527	-5.406255	2.821246
6	3.768206	-5.620637	3.143173

6	-3.847524	4.974829	-0.708615
6	-2.668813	6.422646	1.016170
6	-1.305316	5.406434	2.820955
6	-3.767941	5.620869	3.143239
6	-3.651274	-2.810497	-2.445789
6	-2.863573	-4.945881	-1.304387
6	-0.741544	-4.117860	-0.216227
6	-2.611940	-5.037780	1.163333
6	2.824587	4.100233	-2.565605
6	3.295832	1.922642	-3.648193
6	5.153790	3.135920	-2.502619
1	2.310784	5.887012	-1.456358
1	3.904824	5.230981	-1.079556
1	0.296059	5.126606	-0.247887
1	0.311282	3.575067	0.640144
1	0.439095	3.571435	-1.121631
1	2.295933	6.081999	1.013608
1	3.694794	5.030785	1.359136
1	2.096895	4.667031	2.059534
6	5.239277	-4.795457	-1.332542
6	3.856274	-6.293709	0.079300
6	2.805176	-5.045526	-1.838368
1	1.730834	-6.346956	0.440629
1	2.660096	-7.414195	1.496664

1	1.117867	-6.437659	3.157381
1	0.491035	-5.112731	2.143995
1	1.265992	-4.761497	3.710417
1	4.768778	-5.598931	2.689286
1	3.749767	-4.856365	3.934660
1	3.616396	-6.605803	3.611857
6	-5.239491	4.795362	-1.332418
6	-3.856411	6.293680	0.079270
6	-2.805394	5.045293	-1.838320
1	-1.730937	6.347026	0.440385
1	-2.660131	7.414290	1.496450
1	-1.265657	4.761765	3.710185
1	-0.490937	5.112825	2.143603
1	-1.117579	6.437869	3.156956
1	-3.749376	4.856677	3.934800
1	-3.616067	6.606084	3.611798
1	-4.768582	5.599111	2.689505
6	-2.824803	-4.100248	-2.565010
6	-3.296952	-1.922863	-3.647631
6	-5.154257	-3.136520	-2.501433
1	-2.310365	-5.886896	-1.455843
1	-3.904536	-5.231318	-1.078845
1	-0.295785	-5.126207	-0.247424
1	-0.311154	-3.574566	0.640411

1	-0.439161	-3.571181	-1.121357
1	-2.096570	-4.666759	2.060083
1	-3.694428	-5.030856	1.359775
1	-2.295389	-6.081833	1.014250
1	1.781099	3.833598	-2.800480
1	3.197000	4.677585	-3.427166
1	2.265301	1.546002	-3.567911
1	3.377844	2.511385	-4.574701
1	3.971553	1.062218	-3.749620
1	5.748643	2.214311	-2.419866
1	5.405032	3.625931	-3.456587
1	5.456327	3.797969	-1.679084
1	5.999139	-4.627700	-0.555059
1	5.512192	-5.703943	-1.891499
1	5.276850	-3.952868	-2.036753
1	4.791713	-6.359217	0.658803
1	3.878062	-7.131472	-0.636020
1	3.049040	-5.863556	-2.534259
1	1.793212	-5.211729	-1.443438
1	2.784636	-4.103995	-2.406778
1	-5.999348	4.627713	-0.554906
1	-5.512378	5.703807	-1.891455
1	-5.277114	3.952712	-2.036553
1	-4.791797	6.359216	0.658856

1	-3.878280	7.131384	-0.636116
1	-3.049216	5.863292	-2.534264
1	-1.793410	5.211445	-1.443423
1	-2.784939	4.103718	-2.406659
1	-1.781420	-3.833319	-2.800022
1	-3.197182	-4.677690	-3.426524
1	-2.266490	-1.545961	-3.567702
1	-3.972923	-1.062616	-3.748906
1	-3.379112	-2.511688	-4.574073
1	-5.749295	-2.215030	-2.418669
1	-5.405645	-3.626741	-3.455255
1	-5.456427	-3.798497	-1.677708

Table S4

[Sb-Rea]³

E : -3034.32824008 Hartree

G : -3032.998097 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
51	0.000057	0.000145	0.035947
6	0.000177	0.000022	2.229893

6	1.192672	-0.033684	2.973697
6	-1.192213	0.033679	2.973877
6	2.616775	-0.135881	2.438717
6	1.196331	-0.018712	4.374427
6	-2.616416	0.135880	2.439149
6	-1.195641	0.018701	4.374612
6	3.484394	0.166979	3.700219
6	2.944495	0.805227	1.293030
6	2.904640	-1.487591	1.789413
6	2.598671	-0.024512	4.959143
6	0.000401	0.000001	5.088958
6	-3.483810	-0.167003	3.700797
6	-2.904417	1.487604	1.789941
6	-2.944376	-0.805200	1.293506
6	-2.597882	0.024562	4.959560
1	4.391556	-0.453721	3.723099
1	3.808608	1.216615	3.644284
6	3.505947	0.117843	0.208434
6	2.662068	2.154240	1.192199
6	3.484966	-1.320896	0.520753
6	2.614903	-2.759343	2.247530
6	2.789315	1.136260	5.942332
6	2.898500	-1.344786	5.682106
1	0.000486	0.000015	6.183160

1	-4.390992	0.453663	3.723817
1	-3.807992	-1.216653	3.644936
6	-3.485022	1.320942	0.521405
6	-2.614601	2.759342	2.248046
6	-3.506076	-0.117790	0.209055
6	-2.661970	-2.154212	1.192578
6	-2.788378	-1.136136	5.942864
6	-2.897570	1.344900	5.682463
6	3.804612	0.804876	-0.960104
6	2.901284	2.851759	-0.003808
1	2.170059	2.655828	2.029586
6	3.798261	-2.432241	-0.247854
6	2.933878	-3.899269	1.485685
1	2.103580	-2.877233	3.203957
1	2.525408	2.094551	5.471114
1	2.157969	1.007820	6.834802
1	3.837325	1.189459	6.275673
1	2.177673	-1.515053	6.496192
1	3.909048	-1.320292	6.118154
1	2.848084	-2.200888	4.996325
6	-3.798487	2.432308	-0.247101
6	-2.933734	3.899289	1.486298
1	-2.103097	2.877200	3.204381
6	-3.805006	-0.804795	-0.959432

6	-2.901443	-2.851696	-0.003396
1	-2.169766	-2.655819	2.029840
1	-2.524559	-2.094465	5.471674
1	-2.156884	-1.007637	6.835221
1	-3.836333	-1.189297	6.276380
1	-2.176610	1.515220	6.496421
1	-3.908050	1.320465	6.118673
1	-2.847244	2.200944	4.996601
6	3.493896	2.169648	-1.091741
1	4.238900	0.265304	-1.803288
6	2.372689	4.284689	-0.112316
6	3.547285	-3.732522	0.224361
1	4.223377	-2.291767	-1.243645
6	2.653238	-5.277303	2.095342
6	-3.547404	3.732574	0.225097
1	-4.223822	2.291865	-1.242803
6	-2.652975	5.277311	2.095932
6	-3.494305	-2.169560	-1.091177
1	-4.239494	-0.265203	-1.802499
6	-2.372851	-4.284615	-0.112060
6	3.840051	2.870680	-2.410852
6	3.023390	5.009851	-1.298218
6	0.845737	4.205956	-0.308128
6	2.664343	5.097823	1.156337

6	3.882282	-4.909532	-0.699638
6	2.663639	-6.353308	1.000377
6	1.284454	-5.330888	2.789031
6	3.739795	-5.570509	3.145845
6	-3.882608	4.909601	-0.698801
6	-2.663604	6.353339	1.000991
6	-1.284048	5.330892	2.789336
6	-3.739314	5.570493	3.146667
6	-3.840748	-2.870562	-2.410228
6	-3.023796	-5.009752	-1.297843
6	-0.845944	-4.205854	-0.308211
6	-2.664217	-5.097781	1.156638
6	3.030430	4.167675	-2.561612
6	3.521273	1.984332	-3.623754
6	5.346896	3.183036	-2.411761
1	2.488483	5.957724	-1.470929
1	4.056645	5.282227	-1.025885
1	0.414073	5.220033	-0.350486
1	0.371281	3.660125	0.523338
1	0.577804	3.671364	-1.231230
1	2.367180	6.145998	0.997051
1	3.737051	5.077000	1.399723
1	2.106137	4.730213	2.028443
6	5.278624	-4.751543	-1.318841

6	3.865071	-6.232936	0.080070
6	2.840693	-4.953012	-1.831621
1	1.734495	-6.267206	0.412251
1	2.639356	-7.346356	1.477230
1	1.082554	-6.361949	3.117917
1	0.482668	-5.028194	2.100743
1	1.237207	-4.689438	3.680113
1	4.746991	-5.556653	2.706512
1	3.717202	-4.809439	3.940282
1	3.571545	-6.556208	3.607748
6	-5.279087	4.751611	-1.317694
6	-3.865226	6.232990	0.080928
6	-2.841272	4.953101	-1.831015
1	-1.734582	6.267249	0.412671
1	-2.639220	7.346377	1.477860
1	-1.236612	4.689440	3.680407
1	-0.482411	5.028198	2.100876
1	-1.082075	6.361952	3.118181
1	-3.716545	4.809416	3.941094
1	-3.570979	6.556189	3.608543
1	-4.746602	5.556628	2.707545
6	-3.031127	-4.167533	-2.561207
6	-3.522266	-1.984176	-3.623181
6	-5.347585	-3.182954	-2.410805

1	-2.488901	-5.957606	-1.470701
1	-4.056985	-5.282165	-1.025298
1	-0.414265	-5.219921	-0.350672
1	-0.371313	-3.660019	0.523153
1	-0.578228	-3.671249	-1.231368
1	-2.105811	-4.730195	2.028624
1	-3.736870	-5.076959	1.400270
1	-2.367097	-6.145954	0.997256
1	1.995572	3.910172	-2.840745
1	3.443311	4.743534	-3.405510
1	2.485074	1.616927	-3.580092
1	3.641706	2.570755	-4.547552
1	4.192260	1.117592	-3.699450
1	5.930608	2.256891	-2.304163
1	5.637650	3.667721	-3.357141
1	5.624021	3.845443	-1.579601
1	6.039355	-4.601323	-0.538615
1	5.536876	-5.661908	-1.881621
1	5.333296	-3.906648	-2.019128
1	4.792275	-6.313139	0.670921
1	3.885737	-7.066519	-0.640189
1	3.065401	-5.775528	-2.528771
1	1.823977	-5.094132	-1.438563
1	2.844973	-4.009869	-2.397692

1	-6.039643	4.601384	-0.537300
1	-5.537467	5.661977	-1.880413
1	-5.333910	3.906717	-2.017972
1	-4.792310	6.313188	0.671970
1	-3.886037	7.066585	-0.639312
1	-3.066132	5.775636	-2.528095
1	-1.824468	5.094208	-1.438178
1	-2.845682	4.009973	-2.397107
1	-1.996336	-3.909990	-2.840551
1	-3.444173	-4.743374	-3.405037
1	-2.486067	-1.616742	-3.579742
1	-4.193293	-1.117453	-3.698706
1	-3.642889	-2.570579	-4.546965
1	-5.931291	-2.256824	-2.303052
1	-5.638542	-3.667621	-3.356131
1	-5.624507	-3.845387	-1.578598

Table S5

[Bi-Rea]³

E : -3008.66842200 Hartree

G : -3007.339454 Hartree

Atomic

Coordinates (Angstroms)

Number	X	Y	Z
83	-0.000525	0.000063	-0.065974
6	0.001076	0.000235	2.237067
6	1.192643	-0.027945	2.977586
6	-1.189522	0.028557	2.979136
6	2.617499	-0.121619	2.441257
6	1.198384	-0.012971	4.379182
6	-2.615054	0.122079	2.444638
6	-1.193452	0.013934	4.380741
6	3.484518	0.186515	3.702125
6	2.937865	0.822238	1.296111
6	2.915212	-1.470385	1.790630
6	2.601561	-0.012652	4.961923
6	0.002931	0.000587	5.094682
6	-3.480454	-0.185785	3.706697
6	-2.913673	1.470697	1.794127
6	-2.936961	-0.822044	1.300151
6	-2.595876	0.013752	4.965303
1	4.396667	-0.426987	3.723802
1	3.800394	1.238771	3.646883
6	3.507504	0.140683	0.212027
6	2.638617	2.167370	1.193025
6	3.497069	-1.298512	0.523223

6	2.632817	-2.744880	2.245800
6	2.788118	1.146475	5.947799
6	2.909850	-1.333122	5.680971
1	0.003643	0.000724	6.188937
1	-4.392605	0.427677	3.729387
1	-3.796347	-1.238070	3.652133
6	-3.497227	1.298531	0.527543
6	-2.630754	2.745300	2.248675
6	-3.508043	-0.140731	0.216673
6	-2.637948	-2.167224	1.197004
6	-2.781116	-1.145105	5.951743
6	-2.903268	1.334422	5.684369
6	3.799487	0.830130	-0.957012
6	2.869263	2.866328	-0.003879
1	2.138499	2.662977	2.029105
6	3.819006	-2.406490	-0.246761
6	2.961322	-3.881567	1.483037
1	2.119873	-2.867241	3.200782
1	2.517875	2.104497	5.479628
1	2.159065	1.012203	6.841029
1	3.836477	1.204615	6.279382
1	2.191002	-1.509414	6.495517
1	3.920951	-1.304551	6.115610
1	2.862839	-2.187641	4.992950

6	-3.820326	2.406343	-0.242201
6	-2.960403	3.881817	1.486152
1	-2.116540	2.867875	3.202948
6	-3.801658	-0.830456	-0.951795
6	-2.870280	-2.866478	0.000602
1	-2.136753	-2.662661	2.032540
1	-2.511458	-2.103248	5.483483
1	-2.150898	-1.010565	6.844111
1	-3.829039	-1.203178	6.284711
1	-2.183363	1.510982	6.497925
1	-3.913799	1.305946	6.120337
1	-2.857188	2.188739	4.996036
6	3.471298	2.190708	-1.090737
1	4.240844	0.294854	-1.799332
6	2.319992	4.291257	-0.114824
6	3.576052	-3.709147	0.223140
1	4.245504	-2.261731	-1.241417
6	2.689622	-5.262445	2.090254
6	-3.576849	3.709106	0.227130
1	-4.248208	2.261365	-1.236231
6	-2.687971	5.262837	2.092722
6	-3.473763	-2.191099	-1.085608
1	-4.244146	-0.295365	-1.793639
6	-2.321310	-4.291502	-0.110703

6	3.807450	2.894380	-2.411022
6	2.959077	5.023539	-1.302663
6	0.794125	4.190003	-0.309094
6	2.601013	5.110934	1.152010
6	3.921888	-4.882463	-0.701640
6	2.708453	-6.336497	0.993517
6	1.320668	-5.326635	2.782595
6	3.777217	-5.549715	3.141321
6	-3.924103	4.882213	-0.697386
6	-2.708312	6.336630	0.995754
6	-1.318101	5.327275	2.783225
6	-3.774184	5.550300	3.145162
6	-3.811918	-2.895159	-2.405172
6	-2.962073	-5.024064	-1.297462
6	-0.795698	-4.190458	-0.307083
6	-2.600674	-5.110824	1.156731
6	2.978568	4.178888	-2.564250
6	3.501846	2.001341	-3.622403
6	5.309517	3.228819	-2.412630
1	2.409925	5.962872	-1.477311
1	3.988179	5.312059	-1.031315
1	0.347341	5.197501	-0.351438
1	0.327906	3.637256	0.522708
1	0.533616	3.652110	-1.232713

1	2.286896	6.154025	0.991763
1	3.674418	5.107458	1.393156
1	2.050691	4.735743	2.025817
6	5.319250	-4.714137	-1.315854
6	3.910792	-6.207443	0.075580
6	2.884550	-4.931109	-1.837291
1	1.779808	-6.254903	0.403918
1	2.689257	-7.330513	1.468585
1	1.125535	-6.359599	3.109596
1	0.517555	-5.028263	2.094026
1	1.268125	-4.686903	3.674580
1	4.784779	-5.527728	2.703155
1	3.748187	-4.790230	3.937046
1	3.615612	-6.537435	3.601293
6	-5.322363	4.713671	-1.309497
6	-3.911929	6.207367	0.079521
6	-2.888460	4.930676	-1.834592
1	-1.780489	6.254877	0.404877
1	-2.688439	7.330762	1.470551
1	-1.264315	4.687741	3.675279
1	-0.515894	5.028818	2.093644
1	-1.122611	6.360326	3.109737
1	-3.744002	4.791061	3.941078
1	-3.612059	6.538173	3.604617

1	-4.782332	5.528078	2.708360
6	-2.983298	-4.179738	-2.559238
6	-3.508153	-2.002520	-3.617301
6	-5.314002	-3.229545	-2.404384
1	-2.413189	-5.963457	-1.472630
1	-3.990802	-5.312497	-1.024612
1	-0.349050	-5.198006	-0.349623
1	-0.328331	-3.637414	0.523877
1	-0.536393	-3.652960	-1.231270
1	-2.049182	-4.735392	2.029697
1	-3.673756	-5.107256	1.399304
1	-2.286793	-6.153968	0.996364
1	1.947567	3.905351	-2.842667
1	3.382505	4.759118	-3.409480
1	2.470682	1.619603	-3.578503
1	3.614053	2.587513	-4.547387
1	4.184809	1.143858	-3.696290
1	5.906760	2.311542	-2.303424
1	5.593184	3.716226	-3.358763
1	5.576783	3.896527	-1.581512
1	6.076261	-4.560282	-0.532734
1	5.585471	-5.621751	-1.879381
1	5.370738	-3.867555	-2.014364
1	4.837281	-6.283454	0.668062

1	3.937681	-7.039550	-0.646190
1	3.117622	-5.750291	-2.535619
1	1.867665	-5.080819	-1.447855
1	2.883746	-3.986627	-2.401214
1	-6.078219	4.559982	-0.525229
1	-5.589449	5.621134	-1.872860
1	-5.374841	3.866911	-2.007719
1	-4.837592	6.283511	0.673273
1	-3.939825	7.039309	-0.642400
1	-3.122685	5.749625	-2.532807
1	-1.871021	5.080642	-1.446715
1	-2.888368	3.986031	-2.398244
1	-1.952678	-3.906309	-2.839174
1	-3.388449	-4.760177	-3.403744
1	-2.476923	-1.620772	-3.575116
1	-4.191224	-1.145058	-3.690433
1	-3.621779	-2.588997	-4.541918
1	-5.911035	-2.312197	-2.294631
1	-5.599121	-3.717308	-3.349899
1	-5.580043	-3.896911	-1.572601

Table S6

HCCPh

E : -465.091555287 Hartree

G : -464.905333 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	-2.764503	0.509830	-0.639605
1	-2.557343	-0.478623	-0.274941
6	-2.997927	1.624149	-1.050576
6	-3.275971	2.948857	-1.536455
6	-3.858749	3.912008	-0.697143
1	-4.100584	3.646182	0.332500
6	-4.123858	5.188304	-1.173700
1	-4.577750	5.914626	-0.496447
6	-3.823867	5.560279	-2.494400
6	-3.243363	4.591766	-3.321115
1	-2.991629	4.830098	-4.353821
6	-2.972193	3.306964	-2.855067
1	-2.519315	2.568179	-3.517243
6	-4.136810	6.981591	-2.970968
6	-5.646543	7.239547	-2.834453
1	-6.220210	6.525922	-3.443994
1	-5.889190	8.258427	-3.173134
1	-5.981829	7.141463	-1.792110

6	-3.363022	7.987941	-2.103221
1	-3.642399	7.908202	-1.042990
1	-3.577497	9.016090	-2.432767
1	-2.279195	7.817737	-2.182248
6	-3.738573	7.196360	-4.433725
1	-2.659333	7.047126	-4.585302
1	-3.980461	8.226375	-4.733551
1	-4.281433	6.514878	-5.105188

Table S7

[N-Rea]¹

E : -2848.70258950 Hartree

G : -2847.368408 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	-0.000385	-0.000354	0.976474
6	-0.003616	-0.000503	2.276514
6	1.187317	-0.217506	3.054651
6	-1.198417	0.216324	3.048761
6	2.563350	-0.376011	2.455359
6	1.194072	-0.101571	4.433649

6	-2.571432	0.375175	2.442661
6	-1.212080	0.099908	4.427681
6	3.484986	-0.110328	3.686956
6	2.744568	0.555930	1.265978
6	2.759506	-1.736958	1.782540
6	2.613734	-0.145492	4.982871
6	-0.010797	-0.000965	5.147167
6	-3.499199	0.108841	3.669501
6	-2.764227	1.736490	1.769591
6	-2.746750	-0.556127	1.251904
6	-2.634478	0.143583	4.969787
1	4.311186	-0.833901	3.729599
1	3.932291	0.888263	3.575143
6	3.054369	-0.152309	0.097268
6	2.449321	1.904246	1.202353
6	3.105644	-1.583670	0.429712
6	2.635673	-3.004404	2.317078
6	2.889554	1.084880	5.855478
6	2.850969	-1.413767	5.811686
1	-0.013512	-0.001164	6.241196
1	-4.325769	0.832209	3.708279
1	-3.945706	-0.889807	3.555017
6	-3.103718	1.583883	0.415001
6	-2.643025	3.003683	2.305340

6	-3.050808	0.152700	0.082065
6	-2.450988	-1.904377	1.189012
6	-2.914581	-1.087146	5.840536
6	-2.875936	1.411493	5.797936
6	3.095366	0.513098	-1.118962
6	2.424881	2.579739	-0.028923
1	2.140518	2.425363	2.112481
6	3.366456	-2.701454	-0.347174
6	2.885613	-4.152221	1.539168
1	2.324288	-3.121058	3.356065
1	2.680617	2.011794	5.301077
1	2.262673	1.077526	6.760325
1	3.943419	1.101597	6.173266
1	2.160289	-1.454440	6.667822
1	3.879601	-1.430463	6.202716
1	2.698776	-2.321517	5.212152
6	-3.360674	2.702047	-0.362623
6	-2.889188	4.151883	1.526785
1	-2.336729	3.119843	3.345890
6	-3.085724	-0.512062	-1.134722
6	-2.420280	-2.579176	-0.042491
1	-2.146538	-2.425908	2.100370
1	-2.702695	-2.013827	5.286868
1	-2.292288	-1.080036	6.748547

1	-3.970044	-1.104115	6.152965
1	-2.189568	1.451794	6.657550
1	-3.906517	1.427976	6.183807
1	-2.720776	2.319522	5.199594
6	2.761254	1.876112	-1.206173
1	3.324639	-0.046788	-2.026861
6	1.862960	4.002785	-0.037215
6	3.286499	-3.996961	0.195620
1	3.637390	-2.571633	-1.397088
6	2.746107	-5.522649	2.210190
6	-3.283411	3.997287	0.181188
1	-3.626369	2.572731	-1.413937
6	-2.753193	5.521967	2.199221
6	-2.751036	-1.874978	-1.221006
1	-3.310484	0.048325	-2.043435
6	-1.857634	-4.001953	-0.048750
6	2.770663	2.546883	-2.584587
6	2.169741	4.701427	-1.368710
6	0.341014	3.893298	0.171611
6	2.454233	4.858011	1.091969
6	3.624885	-5.178961	-0.722679
6	2.678254	-6.623902	1.142034
6	1.466357	-5.608919	3.056104
6	3.954327	-5.746398	3.136847

6	-3.617120	5.179748	-0.738226
6	-2.679927	6.623766	1.131994
6	-1.477819	5.607894	3.051743
6	-3.966166	5.745159	3.119791
6	-2.753708	-2.545212	-2.599700
6	-2.156779	-4.699979	-1.382312
6	-0.336865	-3.891763	0.168254
6	-2.454470	-4.858216	1.076715
6	1.896961	3.811316	-2.568070
6	2.210974	1.616464	-3.670828
6	4.222997	2.905161	-2.944351
1	1.569197	5.623904	-1.430294
1	3.225802	5.018831	-1.373091
1	-0.112106	4.897013	0.218428
1	0.106711	3.368099	1.110665
1	-0.149849	3.324341	-0.631631
1	2.102599	5.896492	0.987687
1	3.553787	4.861414	1.052177
1	2.146002	4.508572	2.087420
6	4.960469	-4.935801	-1.442800
6	3.763437	-6.475489	0.090764
6	2.521275	-5.341321	-1.781991
1	1.686248	-6.589889	0.659678
1	2.748966	-7.605633	1.637306

1	1.338870	-6.638946	3.423254
1	0.580238	-5.342150	2.462293
1	1.501087	-4.950951	3.935981
1	4.904582	-5.707174	2.586326
1	3.991179	-4.965583	3.911381
1	3.878968	-6.724392	3.638001
6	-4.949051	4.937018	-1.465227
6	-3.759738	6.475892	0.075127
6	-2.508149	5.342561	-1.791858
1	-1.685479	6.590020	0.654677
1	-2.753195	7.605240	1.627404
1	-1.517102	4.949617	3.931194
1	-0.588678	5.341287	2.462400
1	-1.352181	6.637786	3.419905
1	-4.006857	4.964003	3.893790
1	-3.893490	6.722947	3.621745
1	-4.913600	5.706044	2.564422
6	-1.878805	-3.808750	-2.579651
6	-2.190234	-1.613922	-3.683214
6	-4.204120	-2.904776	-2.965919
1	-1.554881	-5.621735	-1.441409
1	-3.212429	-5.018597	-1.392436
1	0.116510	-4.895265	0.216998
1	-0.107827	-3.366879	1.108778

1	0.157971	-3.322173	-0.632097
1	-2.151906	-4.509143	2.074032
1	-3.553789	-4.862317	1.030931
1	-2.101594	-5.896409	0.973753
1	0.836566	3.509097	-2.569772
1	2.063589	4.366538	-3.505336
1	1.228923	1.216690	-3.377315
1	2.089927	2.180523	-4.608405
1	2.878861	0.770653	-3.885061
1	4.847513	1.999600	-2.958869
1	4.268087	3.372814	-3.940729
1	4.663840	3.597070	-2.213004
1	5.757984	-4.704320	-0.721436
1	5.249419	-5.840988	-1.999235
1	4.900821	-4.109467	-2.164643
1	4.751481	-6.489606	0.579081
1	3.751712	-7.330718	-0.603803
1	2.795366	-6.132360	-2.497345
1	1.556313	-5.604940	-1.327369
1	2.376536	-4.406056	-2.343236
1	-5.750223	4.705189	-0.748039
1	-5.235154	5.842512	-2.022631
1	-4.885784	4.111073	-2.187208
1	-4.750254	6.489824	0.558417

1	-3.744442	7.331457	-0.618957
1	-2.778528	6.134045	-2.508133
1	-1.545448	5.605783	-1.332235
1	-2.360715	4.407591	-2.352890
1	-0.818741	-3.505381	-2.575743
1	-2.040089	-4.363510	-3.518125
1	-1.209837	-1.213282	-3.385382
1	-2.858025	-0.768707	-3.900081
1	-2.064610	-2.177571	-4.620433
1	-4.829318	-1.999734	-2.983183
1	-4.244383	-3.372444	-3.962501
1	-4.647628	-3.597058	-2.236543

Table S8

[P-Rea]¹

E : -3135.35190422 Hartree

G : -3134.017639 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
15	0.284028	0.399635	0.565060
6	-0.094841	0.071662	2.339309

6	1.030030	-0.279828	3.065627
6	-1.275030	0.188841	3.073620
6	2.330132	-0.435779	2.353922
6	1.117886	-0.243614	4.449755
6	-2.661567	0.398747	2.505297
6	-1.269748	0.037670	4.463672
6	3.303757	0.065630	3.465504
6	2.172508	0.326137	1.043554
6	2.696436	-1.804321	1.773547
6	2.594441	-0.182107	4.850590
6	-0.068115	-0.112696	5.179311
6	-3.566743	0.083737	3.737301
6	-2.890051	1.768432	1.864620
6	-2.845674	-0.512105	1.296881
6	-2.683937	0.108635	5.023850
1	4.291220	-0.415103	3.413508
1	3.446994	1.149650	3.332212
6	3.016173	-0.279101	0.013036
6	1.688910	1.700485	0.905531
6	3.213027	-1.665870	0.466989
6	2.558804	-3.065726	2.319852
6	2.833527	1.003536	5.791272
6	3.085874	-1.463473	5.535057
1	-0.069644	-0.107404	6.273413

1	-4.413320	0.781791	3.804227
1	-3.985602	-0.924945	3.605836
6	-3.297789	1.633071	0.524801
6	-2.723099	3.033965	2.395055
6	-3.209524	0.211542	0.156239
6	-2.484807	-1.842756	1.185710
6	-2.982382	-1.106384	5.909599
6	-2.894942	1.389217	5.842148
6	3.315284	0.415800	-1.102115
6	2.123798	2.436008	-0.306369
1	1.507514	2.273974	1.818273
6	3.637962	-2.789023	-0.227590
6	2.955170	-4.217029	1.612158
1	2.086353	-3.174754	3.296941
1	2.438996	1.933984	5.357119
1	2.339438	0.841533	6.761565
1	3.910799	1.134681	5.977420
1	2.486146	-1.673121	6.433669
1	4.136887	-1.353210	5.843035
1	3.021821	-2.332595	4.869037
6	-3.625821	2.754969	-0.219921
6	-3.021124	4.187388	1.641622
1	-2.336584	3.144645	3.409566
6	-3.239562	-0.417850	-1.081816

6	-2.444286	-2.478176	-0.065985
1	-2.133453	-2.372689	2.074684
1	-2.790949	-2.042866	5.365129
1	-2.353184	-1.101055	6.812717
1	-4.035626	-1.100262	6.230441
1	-2.196348	1.426997	6.691781
1	-3.920624	1.428232	6.240015
1	-2.731891	2.287530	5.231532
6	2.828884	1.793860	-1.286521
1	3.917274	-0.038567	-1.890245
6	1.683075	3.895560	-0.369406
6	3.534646	-4.073800	0.333553
1	4.017840	-2.673213	-1.244959
6	2.750924	-5.578676	2.283812
6	-3.535016	4.043401	0.336186
1	-3.962800	2.633918	-1.251853
6	-2.770403	5.552735	2.289163
6	-2.835831	-1.755770	-1.217598
1	-3.510832	0.158118	-1.967961
6	-1.822221	-3.875895	-0.136104
6	3.159995	2.446657	-2.630079
6	2.336833	4.596715	-1.568400
6	0.148499	3.968895	-0.465900
6	2.124349	4.644284	0.900803

6	3.993786	-5.264937	-0.516018
6	2.852154	-6.700700	1.240598
6	1.366522	-5.676234	2.943347
6	3.823206	-5.758646	3.372693
6	-4.010332	5.227466	-0.515360
6	-2.855394	6.660387	1.228722
6	-1.364193	5.607638	2.905732
6	-3.806549	5.791072	3.400164
6	-2.831858	-2.374696	-2.620503
6	-2.163847	-4.547113	-1.473115
6	-0.295940	-3.715938	0.010384
6	-2.330342	-4.784418	0.991643
6	2.331848	3.727106	-2.811259
6	2.796012	1.498894	-3.785935
6	4.663668	2.758207	-2.698512
1	1.813635	5.548669	-1.753284
1	3.375651	4.857860	-1.306859
1	-0.172859	5.022284	-0.422601
1	-0.339756	3.432020	0.363153
1	-0.225289	3.528824	-1.402714
1	1.929489	5.720667	0.773270
1	3.201174	4.510094	1.084465
1	1.575203	4.318249	1.795076
6	5.393596	-5.012384	-1.095482

6	4.060942	-6.541702	0.335607
6	3.006153	-5.462576	-1.679167
1	1.930631	-6.703805	0.633678
1	2.882893	-7.670285	1.762952
1	1.200339	-6.706319	3.294220
1	0.569576	-5.422004	2.229277
1	1.269563	-5.014942	3.815745
1	4.839403	-5.718747	2.956216
1	3.743769	-4.958790	4.124186
1	3.691674	-6.725051	3.884370
6	-5.423475	4.953525	-1.054133
6	-4.071425	6.506926	0.333267
6	-3.063784	5.434483	-1.708565
1	-1.939174	6.631836	0.614344
1	-2.861363	7.639159	1.734479
1	-1.254381	4.926498	3.761402
1	-0.602271	5.345304	2.156856
1	-1.157671	6.627470	3.265804
1	-3.743318	5.000524	4.162818
1	-3.624428	6.758586	3.893751
1	-4.832889	5.787528	3.006926
6	-1.938229	-3.624558	-2.657482
6	-2.286200	-1.389762	-3.665658
6	-4.277024	-2.744949	-2.996219

1	-1.556364	-5.460967	-1.576435
1	-3.216719	-4.874730	-1.449869
1	0.201267	-4.699878	-0.028874
1	-0.042276	-3.243822	0.972959
1	0.131458	-3.078040	-0.777350
1	-1.996400	-4.447582	1.983004
1	-3.429465	-4.833713	0.995561
1	-1.940542	-5.803996	0.844754
1	1.294481	3.443874	-3.056012
1	2.719240	4.283241	-3.680078
1	1.758889	1.144420	-3.687956
1	2.888158	2.036171	-4.742507
1	3.455807	0.621917	-3.837082
1	5.260627	1.848827	-2.533702
1	4.926342	3.162524	-3.688609
1	4.958839	3.489688	-1.933128
1	6.108936	-4.764540	-0.297486
1	5.749767	-5.918631	-1.609404
1	5.400139	-4.193338	-1.828077
1	4.977892	-6.517735	0.946943
1	4.160783	-7.409469	-0.335850
1	3.343402	-6.283852	-2.330597
1	1.995651	-5.699063	-1.316863
1	2.931076	-4.549604	-2.288068

1	-6.112600	4.701973	-0.234596
1	-5.805349	5.851419	-1.564552
1	-5.438091	4.127475	-1.778810
1	-4.983264	6.484742	0.952473
1	-4.175024	7.373783	-0.338743
1	-3.451065	6.227994	-2.366457
1	-2.054685	5.718439	-1.380904
1	-2.970638	4.512855	-2.301834
1	-0.882910	-3.307000	-2.680652
1	-2.121528	-4.158862	-3.603688
1	-1.314587	-0.982204	-3.348215
1	-2.969833	-0.549311	-3.849114
1	-2.147844	-1.912489	-4.624626
1	-4.921681	-1.854049	-2.966810
1	-4.313326	-3.164878	-4.013877
1	-4.700866	-3.481531	-2.299043

Table S9

[As-Rea]¹

E : -5029.74123591 Hartree

G : -5028.409565 Hartree

Atomic

Coordinates (Angstroms)

Number	X	Y	Z
33	0.196257	0.464774	0.426989
6	-0.125628	0.098607	2.319953
6	1.030549	-0.208224	3.018708
6	-1.290296	0.169606	3.083831
6	2.331201	-0.363274	2.302491
6	1.137027	-0.198224	4.404078
6	-2.693689	0.345667	2.545980
6	-1.254534	0.012720	4.472279
6	3.315864	0.118061	3.414620
6	2.244900	0.415535	1.000026
6	2.678252	-1.739515	1.729846
6	2.613931	-0.137497	4.798124
6	-0.035650	-0.113410	5.160625
6	-3.566754	0.008975	3.794846
6	-2.952510	1.712058	1.911779
6	-2.892834	-0.566019	1.341465
6	-2.657756	0.049233	5.062146
1	4.298428	-0.370888	3.348623
1	3.467893	1.201875	3.290390
6	3.067830	-0.220561	-0.017089
6	1.805512	1.783993	0.851116
6	3.221982	-1.613362	0.434301

6	2.507503	-2.996124	2.277391
6	2.856544	1.042684	5.745301
6	3.108374	-1.422797	5.473438
1	-0.012783	-0.129712	6.254343
1	-4.426051	0.689151	3.881420
1	-3.967513	-1.007784	3.669219
6	-3.388652	1.574191	0.581671
6	-2.758912	2.977578	2.432279
6	-3.303113	0.152290	0.212423
6	-2.522098	-1.893129	1.219723
6	-2.911101	-1.173138	5.951543
6	-2.879448	1.324443	5.886145
6	3.405848	0.465906	-1.131297
6	2.257273	2.509883	-0.346885
1	1.561271	2.352409	1.751021
6	3.636361	-2.744874	-0.252186
6	2.901462	-4.155730	1.581523
1	2.015466	-3.091806	3.246330
1	2.460445	1.975561	5.317856
1	2.364954	0.874830	6.715843
1	3.934377	1.172734	5.929233
1	2.509009	-1.640635	6.370377
1	4.158956	-1.311843	5.782809
1	3.047140	-2.286964	4.800618

6	-3.712734	2.696030	-0.164521
6	-3.049231	4.130781	1.676130
1	-2.347584	3.086605	3.437226
6	-3.374802	-0.481906	-1.021857
6	-2.527541	-2.533800	-0.030135
1	-2.132586	-2.416199	2.096733
1	-2.710676	-2.104407	5.401338
1	-2.263494	-1.155520	6.841398
1	-3.957246	-1.190672	6.294500
1	-2.160988	1.379621	6.718058
1	-3.895762	1.338690	6.309030
1	-2.753910	2.226002	5.271208
6	2.964704	1.850042	-1.321251
1	4.002385	-0.009738	-1.910844
6	1.866767	3.985281	-0.413622
6	3.502257	-4.026146	0.311091
1	4.035714	-2.638581	-1.263087
6	2.681124	-5.511913	2.259281
6	-3.585295	3.986353	0.379342
1	-4.063709	2.574507	-1.191615
6	-2.765072	5.495691	2.311255
6	-2.971489	-1.819274	-1.167613
1	-3.685258	0.088298	-1.898823
6	-1.902613	-3.929414	-0.118276

6	3.342331	2.498919	-2.654441
6	2.583356	4.668394	-1.587041
6	0.340512	4.120695	-0.560306
6	2.294816	4.710348	0.874556
6	3.953428	-5.227123	-0.529250
6	2.770049	-6.638794	1.220356
6	1.297714	-5.594169	2.922121
6	3.753280	-5.697191	3.347681
6	-4.026896	5.174872	-0.482964
6	-2.839253	6.599527	1.245865
6	-1.352103	5.528893	2.913994
6	-3.786212	5.760133	3.430292
6	-3.029313	-2.448843	-2.564518
6	-2.293799	-4.609636	-1.437109
6	-0.372349	-3.763833	-0.033082
6	-2.363457	-4.833316	1.033378
6	2.570603	3.813348	-2.839958
6	2.962404	1.573682	-3.823188
6	4.858238	2.751885	-2.694256
1	2.109008	5.645157	-1.773591
1	3.625798	4.878621	-1.295617
1	0.065333	5.187809	-0.534412
1	-0.194960	3.606768	0.253617
1	-0.020458	3.690522	-1.506498

1	2.145759	5.793931	0.747752
1	3.359062	4.533667	1.092282
1	1.704880	4.400868	1.748482
6	5.364482	-4.999758	-1.091658
6	3.988366	-6.503992	0.324302
6	2.976972	-5.410727	-1.704099
1	1.852882	-6.626987	0.606827
1	2.780031	-7.607280	1.745572
1	1.125811	-6.620103	3.282240
1	0.501171	-5.341809	2.207396
1	1.206742	-4.924975	3.789121
1	4.769632	-5.661799	2.931305
1	3.677437	-4.896749	4.098893
1	3.617263	-6.662844	3.859669
6	-5.441370	4.936356	-1.033876
6	-4.061483	6.460929	0.356576
6	-3.060684	5.344437	-1.666584
1	-1.926672	6.555311	0.627450
1	-2.828653	7.580382	1.747552
1	-1.245316	4.851497	3.772874
1	-0.602805	5.248909	2.158589
1	-1.124084	6.547285	3.265086
1	-3.732380	4.971972	4.196105
1	-3.580382	6.726186	3.917380

1	-4.815689	5.775554	3.045538
6	-2.126957	-3.690889	-2.634184
6	-2.545175	-1.468622	-3.643555
6	-4.487884	-2.834539	-2.866024
1	-1.682820	-5.518429	-1.561783
1	-3.341570	-4.946915	-1.368542
1	0.124452	-4.747999	-0.073658
1	-0.082226	-3.273204	0.909620
1	0.023284	-3.140021	-0.848067
1	-1.995014	-4.488626	2.009660
1	-3.461430	-4.887672	1.078526
1	-1.974332	-5.851961	0.878384
1	1.528425	3.576086	-3.111343
1	3.000125	4.361789	-3.693622
1	1.909334	1.263403	-3.749009
1	3.097558	2.111318	-4.774415
1	3.585056	0.669467	-3.865170
1	5.416726	1.818552	-2.529273
1	5.152467	3.155323	-3.675704
1	5.168734	3.464145	-1.916904
1	6.073713	-4.760922	-0.285477
1	5.712038	-5.913718	-1.597778
1	5.394142	-4.183868	-1.827205
1	4.900825	-6.498408	0.942616

1	4.076084	-7.374093	-0.345830
1	3.307593	-6.239782	-2.349041
1	1.958286	-5.627955	-1.352929
1	2.925323	-4.498355	-2.316279
1	-6.145963	4.712320	-0.219515
1	-5.792012	5.840180	-1.556074
1	-5.472877	4.105021	-1.751863
1	-4.971377	6.458833	0.979210
1	-4.152127	7.324801	-0.321166
1	-3.402472	6.159189	-2.323863
1	-2.041925	5.574730	-1.326672
1	-3.006896	4.422026	-2.263506
1	-1.076574	-3.363689	-2.703879
1	-2.345801	-4.231551	-3.569148
1	-1.561317	-1.051805	-3.380657
1	-3.243640	-0.634648	-3.798312
1	-2.452540	-1.998233	-4.604226
1	-5.137470	-1.948226	-2.814749
1	-4.569851	-3.265704	-3.876291
1	-4.871734	-3.566594	-2.141517

Table S10

[Sb-Rea]¹

E : -3034.29490835 Hartree

G : -3032.965122 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
51	0.000393	-0.000048	0.088042
6	0.000192	-0.000038	2.245081
6	1.182277	-0.052812	2.996859
6	-1.181975	0.052783	2.996756
6	2.582817	-0.173214	2.425144
6	1.195454	-0.009400	4.392097
6	-2.582517	0.173208	2.425000
6	-1.195224	0.009505	4.392006
6	3.479321	0.167450	3.652845
6	2.780256	0.735188	1.223698
6	2.847463	-1.541275	1.795047
6	2.613020	0.039599	4.942318
6	0.000090	0.000087	5.115170
6	-3.479043	-0.167453	3.652680
6	-2.847172	1.541287	1.794949
6	-2.780068	-0.735167	1.223548
6	-2.612817	-0.039343	4.942164
1	4.373858	-0.470842	3.686852

1	3.825171	1.206820	3.549608
6	3.166694	0.009293	0.082963
6	2.555544	2.099584	1.133907
6	3.241675	-1.415899	0.452680
6	2.681702	-2.801234	2.336497
6	2.798378	1.269610	5.839739
6	2.954364	-1.219311	5.749922
1	0.000051	0.000164	6.209042
1	-4.373657	0.470736	3.686580
1	-3.824756	-1.206878	3.549530
6	-3.241514	1.415951	0.452619
6	-2.681345	2.801226	2.336427
6	-3.166611	-0.009240	0.082866
6	-2.555494	-2.099587	1.133733
6	-2.798257	-1.269140	5.839862
6	-2.954172	1.219773	5.749438
6	3.329631	0.673264	-1.130142
6	2.702757	2.780413	-0.084285
1	2.205639	2.633974	2.020659
6	3.530824	-2.543232	-0.299259
6	2.956512	-3.960506	1.586186
1	2.304745	-2.897939	3.355243
1	2.513459	2.187850	5.305015
1	2.176552	1.195124	6.744760

1	3.849122	1.362019	6.156209
1	2.261286	-1.335433	6.596808
1	3.977422	-1.153229	6.151246
1	2.890673	-2.126186	5.133905
6	-3.530676	2.543311	-0.299274
6	-2.956174	3.960527	1.586167
1	-2.304341	2.897882	3.355161
6	-3.329711	-0.673193	-1.130230
6	-2.702907	-2.780399	-0.084443
1	-2.205589	-2.634023	2.020460
1	-2.513316	-2.187512	5.305377
1	-2.176495	-1.194449	6.744910
1	-3.849026	-1.361456	6.156280
1	-2.261127	1.336098	6.596323
1	-3.977250	1.153813	6.150734
1	-2.890440	2.126487	5.133184
6	3.091465	2.054295	-1.234592
1	3.624688	0.105643	-2.014093
6	2.295037	4.254675	-0.128031
6	3.419471	-3.828436	0.258894
1	3.829838	-2.431135	-1.343459
6	2.777436	-5.319308	2.271764
6	-3.419216	3.828498	0.258896
1	-3.829805	2.431247	-1.343445

6	-2.777139	5.319314	2.271797
6	-3.091643	-2.054242	-1.234718
1	-3.624862	-0.105549	-2.014133
6	-2.295444	-4.254728	-0.128181
6	3.279375	2.718917	-2.603303
6	2.829138	4.918792	-1.404365
6	0.756600	4.321586	-0.090863
6	2.850475	5.028223	1.076171
6	3.765188	-5.028947	-0.630432
6	2.756513	-6.440959	1.223366
6	1.455924	-5.386280	3.052023
6	3.937878	-5.529420	3.260452
6	-3.764951	5.029036	-0.630382
6	-2.756352	6.441030	1.223462
6	-1.455594	5.386365	3.051989
6	-3.937538	5.529282	3.260571
6	-3.279826	-2.718885	-2.603388
6	-2.829749	-4.918793	-1.404456
6	-0.757017	-4.321934	-0.091111
6	-2.850947	-5.028120	1.076092
6	2.569582	4.081205	-2.643751
6	2.687531	1.856695	-3.728311
6	4.786551	2.897942	-2.855693
1	2.363969	5.912324	-1.507299

1	3.912240	5.093052	-1.291037
1	0.426599	5.373696	-0.060824
1	0.361181	3.801395	0.795422
1	0.300090	3.829140	-0.961201
1	2.643237	6.101836	0.948468
1	3.939165	4.895678	1.163803
1	2.386740	4.717756	2.022928
6	5.110530	-4.813231	-1.339691
6	3.880811	-6.308399	0.212025
6	2.667770	-5.198802	-1.694581
1	1.784344	-6.418415	0.702492
1	2.810887	-7.412485	1.740275
1	1.312501	-6.406270	3.440757
1	0.603783	-5.143296	2.401037
1	1.439037	-4.702452	3.912121
1	4.913689	-5.506631	2.755362
1	3.942105	-4.733462	4.020179
1	3.832457	-6.496820	3.776315
6	-5.110252	4.813307	-1.339711
6	-3.880653	6.308442	0.212129
6	-2.667476	5.198985	-1.694460
1	-1.784192	6.418608	0.702568
1	-2.810806	7.412520	1.740432
1	-1.438614	4.702536	3.912084

1	-0.603464	5.143450	2.400960
1	-1.312225	6.406361	3.440725
1	-3.941613	4.733316	4.020290
1	-3.832198	6.496692	3.776434
1	-4.913382	5.506377	2.755551
6	-2.570200	-4.081257	-2.643877
6	-2.688040	-1.856803	-3.728535
6	-4.787059	-2.897744	-2.855554
1	-2.364713	-5.912384	-1.507416
1	-3.912863	-5.092917	-1.291029
1	-0.427241	-5.374114	-0.061041
1	-0.361416	-3.801788	0.795120
1	-0.300463	-3.829633	-0.961508
1	-2.387137	-4.717645	2.022810
1	-3.939615	-4.895422	1.163754
1	-2.643856	-6.101770	0.948457
1	1.485931	3.913617	-2.755232
1	2.894457	4.618962	-3.548894
1	1.643725	1.587591	-3.506846
1	2.705768	2.423607	-4.671700
1	3.256112	0.931161	-3.893830
1	5.300981	1.926049	-2.826205
1	4.957058	3.349085	-3.845755
1	5.251302	3.540541	-2.094639

1	5.903767	-4.580903	-0.613910
1	5.393941	-5.730179	-1.879351
1	5.068938	-3.997800	-2.075130
1	4.850384	-6.306349	0.736668
1	3.898606	-7.176942	-0.465714
1	2.919332	-6.027746	-2.374631
1	1.691328	-5.406025	-1.235864
1	2.560603	-4.282124	-2.293369
1	-5.903521	4.580935	-0.613978
1	-5.393664	5.730264	-1.879356
1	-5.068602	3.997902	-2.075174
1	-4.850225	6.306319	0.736772
1	-3.898497	7.177010	-0.465576
1	-2.919026	6.027961	-2.374477
1	-1.691068	5.406213	-1.235672
1	-2.560247	4.282344	-2.293293
1	-1.486539	-3.913798	-2.755458
1	-2.895222	-4.618992	-3.548980
1	-1.644187	-1.587761	-3.507212
1	-3.256568	-0.931241	-3.894080
1	-2.706427	-2.423796	-4.671872
1	-5.301365	-1.925786	-2.826044
1	-4.957763	-3.348921	-3.845567
1	-5.251780	-3.540244	-2.094398

Table S11**[Bi-Rea]¹**

E : -3008.63354730 Hartree

G : -3007.303814 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
83	0.000441	0.000179	-0.033894
6	-0.000928	-0.000258	2.241499
6	1.180517	-0.069466	2.993214
6	-1.183195	0.068634	2.991948
6	2.592517	-0.200226	2.432752
6	1.192698	-0.027986	4.390096
6	-2.594577	0.199683	2.429978
6	-1.196910	0.026583	4.388795
6	3.487188	0.094899	3.671345
6	2.796396	0.732941	1.251895
6	2.833890	-1.557731	1.772892
6	2.604722	0.002068	4.952417
6	-0.002501	-0.000853	5.110742
6	-3.490622	-0.095842	3.667474

6	-2.835066	1.557450	1.770333
6	-2.797134	-0.733046	1.248537
6	-2.609550	-0.003615	4.949550
1	4.348301	-0.587533	3.711693
1	3.888745	1.114871	3.577358
6	3.082000	0.019323	0.074614
6	2.635032	2.106789	1.206076
6	3.152096	-1.414272	0.413207
6	2.723773	-2.825992	2.310260
6	2.805021	1.241170	5.834420
6	2.910551	-1.251340	5.782222
1	-0.003104	-0.001078	6.204794
1	-4.351713	0.586656	3.707158
1	-3.892179	-1.115736	3.572637
6	-3.151538	1.414520	0.410189
6	-2.725556	2.825507	2.308308
6	-3.081070	-0.018948	0.071141
6	-2.635961	-2.106903	1.202423
6	-2.810906	-1.243061	5.830824
6	-2.916191	1.249481	5.779532
6	3.178088	0.702584	-1.137196
6	2.719309	2.807481	-0.006671
1	2.370406	2.636249	2.124653
6	3.401623	-2.530051	-0.370428

6	2.969024	-3.973333	1.532754
1	2.427031	-2.939203	3.353182
1	2.550054	2.157341	5.281251
1	2.167194	1.195799	6.730136
1	3.852641	1.314337	6.166118
1	2.218532	-1.329004	6.634365
1	3.937336	-1.212057	6.177608
1	2.810606	-2.167547	5.184725
6	-3.400084	2.530598	-0.373327
6	-2.969807	3.973153	1.530930
1	-2.430139	2.938311	3.351652
6	-3.175499	-0.701717	-1.141072
6	-2.718648	-2.807119	-0.010720
1	-2.372716	-2.636766	2.121163
1	-2.555435	-2.159029	5.277549
1	-2.174026	-1.198119	6.727236
1	-3.858884	-1.316267	6.161375
1	-2.225104	1.326740	6.632467
1	-3.943413	1.210120	6.173772
1	-2.815512	2.165923	5.182518
6	2.979107	2.092271	-1.199115
1	3.387652	0.142674	-2.050394
6	2.358322	4.293944	0.009482
6	3.335598	-3.822098	0.176793

1	3.637896	-2.401714	-1.428651
6	2.881908	-5.340344	2.219894
6	-3.334775	3.822431	0.174481
1	-3.635074	2.402674	-1.431888
6	-2.883341	5.339908	2.218667
6	-2.976537	-2.091400	-1.203263
1	-3.383692	-0.141429	-2.054353
6	-2.358060	-4.293680	0.005384
6	3.056179	2.774356	-2.569757
6	2.777510	4.964476	-1.305679
6	0.833454	4.394997	0.203173
6	3.056485	5.031821	1.160100
6	3.625016	-5.009808	-0.749541
6	2.797458	-6.455745	1.168171
6	1.637926	-5.447256	3.114047
6	4.130556	-5.525979	3.100587
6	-3.623329	5.010471	-0.751691
6	-2.797816	6.455697	1.167444
6	-1.640205	5.446430	3.114055
6	-4.132823	5.525293	3.098219
6	-3.051434	-2.772851	-2.574346
6	-2.775417	-4.963544	-1.310701
6	-0.833524	-4.395209	0.201382
6	-3.058215	-5.031841	1.154607

6	2.374814	4.151123	-2.522508
6	2.339925	1.944118	-3.645523
6	4.536113	2.924301	-2.961986
1	2.328629	5.969815	-1.348537
1	3.870298	5.112698	-1.300340
1	0.522945	5.453000	0.236225
1	0.528374	3.908877	1.142424
1	0.281932	3.880766	-0.596970
1	2.856333	6.111207	1.077775
1	4.145539	4.880006	1.123321
1	2.695410	4.707353	2.145888
6	4.901739	-4.768577	-1.568868
6	3.830699	-6.294333	0.067707
6	2.444006	-5.189707	-1.718956
1	1.784917	-6.451390	0.730434
1	2.915361	-7.428877	1.671331
1	1.555043	-6.473807	3.503085
1	0.725189	-5.219776	2.545337
1	1.682028	-4.771984	3.979942
1	5.057370	-5.469798	2.512651
1	4.178702	-4.737256	3.866331
1	4.098046	-6.500921	3.612096
6	-4.899235	4.769427	-1.572343
6	-3.829915	6.294670	0.065849

6	-2.441404	5.190821	-1.719901
1	-1.784824	6.451514	0.730751
1	-2.916245	7.428643	1.670840
1	-1.685177	4.770843	3.979657
1	-0.726939	5.219097	2.546132
1	-1.557631	6.472836	3.503541
1	-4.181772	4.736290	3.863621
1	-4.100736	6.500040	3.610127
1	-5.059074	5.469409	2.509364
6	-2.370529	-4.149826	-2.526555
6	-2.333030	-1.942304	-3.648446
6	-4.530706	-2.922210	-2.969267
1	-2.326827	-5.969025	-1.353265
1	-3.868267	-5.111375	-1.307125
1	-0.523272	-5.453293	0.234246
1	-0.529822	-3.909760	1.141423
1	-0.280655	-3.880569	-0.597569
1	-2.698636	-4.707831	2.141091
1	-4.147173	-4.879762	1.116153
1	-2.858179	-6.111241	1.072186
1	1.281708	4.006516	-2.523782
1	2.617867	4.694847	-3.449482
1	1.314251	1.699117	-3.330016
1	2.284294	2.524793	-4.579009

1	2.865909	1.007289	-3.876047
1	5.026746	1.940350	-2.998716
1	4.623155	3.390696	-3.955832
1	5.087173	3.540491	-2.237703
1	5.748435	-4.519650	-0.912271
1	5.156639	-5.680746	-2.130327
1	4.783009	-3.956067	-2.299079
1	4.840744	-6.281076	0.509185
1	3.805355	-7.156429	-0.618056
1	2.657753	-5.998509	-2.435278
1	1.516596	-5.433840	-1.182909
1	2.261508	-4.264758	-2.286459
1	-5.746545	4.520205	-0.916652
1	-5.153661	5.681770	-2.133733
1	-4.779732	3.957172	-2.302712
1	-4.840409	6.281186	0.506292
1	-3.803917	7.157036	-0.619549
1	-2.654521	5.999875	-2.436124
1	-1.514533	5.434822	-1.182868
1	-2.258284	4.266103	-2.287580
1	-1.277383	-4.005522	-2.525997
1	-2.612232	-4.693104	-3.454144
1	-1.307834	-1.697801	-3.331000
1	-2.858305	-1.005188	-3.879422

1	-2.275941	-2.522533	-4.582122
1	-5.021052	-1.938128	-3.006305
1	-4.616099	-3.388015	-3.963531
1	-5.083184	-3.538694	-2.246314

Table S12

[N-TS]³

E : -3313.85538652 Hartree

G : -3312.32141363 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
7	0.199435	-0.672011	-0.200261
6	1.453181	0.802512	0.240453
6	0.826617	1.880966	0.231096
6	0.841954	-1.879819	-0.190386
6	1.630174	-2.348418	-1.265903
6	0.624623	-2.779371	0.879884
6	2.041509	-1.561565	-2.490044
6	2.107268	-3.657543	-1.298586
6	-0.246396	-2.514443	2.090113
6	1.166428	-4.059045	0.875597

6	2.467818	-2.696886	-3.469222
6	3.137750	-0.546539	-2.163311
6	0.956294	-0.642387	-3.028048
6	2.773771	-3.973327	-2.631668
6	1.902786	-4.523603	-0.220703
6	0.043590	-3.759058	2.986851
6	-1.713511	-2.328893	1.698782
6	0.043743	-1.178790	2.763804
6	0.817047	-4.819208	2.145187
1	3.316234	-2.391894	-4.098116
1	1.617992	-2.900111	-4.137934
6	2.782043	0.734181	-2.612409
6	4.281619	-0.712353	-1.403069
6	1.422579	0.672320	-3.167611
6	-0.384339	-0.921479	-3.205575
6	4.279375	-4.228804	-2.481136
6	2.125201	-5.207205	-3.271470
1	2.290743	-5.546016	-0.241582
1	-0.888276	-4.167819	3.402493
1	0.662431	-3.439795	3.837816
6	-2.190658	-1.075147	2.113351
6	-2.559034	-3.196429	1.035169
6	-1.093075	-0.358170	2.778637
6	1.238031	-0.710635	3.277551

6	-0.046725	-6.047873	1.833702
6	2.091254	-5.269073	2.870333
6	3.580870	1.823888	-2.299042
6	5.104242	0.381689	-1.074913
1	4.515695	-1.697493	-0.999095
6	0.562918	1.667482	-3.607966
6	-1.292258	0.102691	-3.526415
1	-0.752958	-1.929970	-2.997160
1	4.465023	-5.054001	-1.776815
1	4.715998	-4.505315	-3.452941
1	4.810740	-3.340211	-2.116926
1	2.333585	-6.114443	-2.683973
1	2.520577	-5.364220	-4.286897
1	1.034177	-5.084603	-3.338124
6	-3.498824	-0.704759	1.835569
6	-3.906232	-2.861639	0.792117
1	-2.178051	-4.162238	0.696475
6	-1.025866	0.907861	3.339389
6	1.332826	0.584964	3.820260
1	2.124952	-1.348816	3.234268
1	0.489035	-6.746230	1.173100
1	-0.302270	-6.582767	2.761116
1	-0.983869	-5.763047	1.335388
1	2.656376	-5.993290	2.263928

1	1.840228	-5.750178	3.828235
1	2.747067	-4.409781	3.074916
6	4.742700	1.671181	-1.525363
1	3.259310	2.822843	-2.600117
6	6.382903	0.117502	-0.274457
6	-0.799184	1.391871	-3.818988
1	0.936130	2.684704	-3.748534
6	-2.786375	-0.213403	-3.423182
6	-4.373134	-1.585188	1.172278
1	-3.852893	0.280882	2.147695
6	-4.795502	-3.926070	0.134434
6	0.175910	1.392111	3.882904
1	-1.914771	1.542761	3.342203
6	2.699500	1.062601	4.320885
6	5.489359	2.939471	-1.096480
6	6.845993	1.408374	0.415722
6	6.169484	-0.944978	0.812328
6	7.463266	-0.393019	-1.244995
6	-1.694431	2.520850	-4.338834
6	-3.204444	-1.206755	-4.517559
6	-3.608800	1.080504	-3.527009
6	-3.071758	-0.833419	-2.045800
6	-5.816368	-1.130056	0.929191
6	-6.275265	-3.516697	0.206497

6	-4.383636	-4.128067	-1.333529
6	-4.646247	-5.268386	0.869241
6	0.163583	2.799180	4.492573
6	2.691277	2.588024	4.493748
6	3.023067	0.368234	5.654536
6	3.802617	0.715763	3.310016
6	6.875718	2.595087	-0.531633
6	5.688440	3.900599	-2.276745
6	4.645133	3.644259	-0.017910
1	7.843450	1.239847	0.852762
1	6.166890	1.619005	1.259342
1	5.305444	-0.692371	1.443368
1	7.061817	-0.996483	1.454796
1	6.011162	-1.949267	0.394828
1	7.133267	-1.328142	-1.722008
1	8.402011	-0.593196	-0.704472
1	7.667658	0.329827	-2.046899
6	-3.103859	1.986097	-4.636352
6	-1.769699	3.643553	-3.294825
6	-1.112874	3.087226	-5.642748
1	-2.610444	-2.130532	-4.454076
1	-4.266208	-1.476909	-4.402254
1	-3.060346	-0.787487	-5.523889
1	-3.551042	1.615792	-2.562859

1	-4.668901	0.819455	-3.678303
1	-2.715079	-0.177702	-1.236561
1	-4.157721	-0.975624	-1.922676
1	-2.592136	-1.813168	-1.909102
6	-6.488233	-2.045883	-0.104509
6	-5.867384	0.308132	0.389598
6	-6.584820	-1.172924	2.261677
1	-6.661976	-3.737822	1.214491
1	-6.850600	-4.148679	-0.488767
1	-3.309671	-4.355216	-1.413335
1	-4.944959	-4.968921	-1.769764
1	-4.578561	-3.231778	-1.937716
1	-4.822515	-5.146161	1.948173
1	-5.381867	-5.987880	0.477238
1	-3.648422	-5.709021	0.732439
6	1.469806	3.072567	5.253370
6	-0.998683	2.947443	5.486176
6	-0.015757	3.830999	3.367990
1	3.617339	2.893090	5.007203
1	2.716351	3.055151	3.494471
1	3.039028	-0.724093	5.524356
1	4.011601	0.685063	6.022937
1	2.273425	0.596206	6.425016
1	3.547193	1.093076	2.307065

1	4.752610	1.178272	3.622615
1	3.974391	-0.367472	3.240954
1	7.278989	3.485105	-0.022340
1	7.561523	2.382401	-1.367989
1	6.184390	3.392988	-3.117242
1	6.321296	4.744558	-1.961582
1	4.739878	4.319548	-2.639821
1	3.640291	3.876102	-0.401280
1	5.127194	4.584507	0.293032
1	4.512808	3.008749	0.870014
1	-3.783130	2.840127	-4.789646
1	-3.084767	1.427332	-5.587272
1	-0.772193	4.053779	-3.079644
1	-2.404299	4.467598	-3.660803
1	-2.178761	3.278071	-2.343103
1	-0.980577	2.291688	-6.390857
1	-1.797671	3.843148	-6.058246
1	-0.138463	3.569832	-5.481476
1	-7.563564	-1.809059	-0.143938
1	-6.081877	-1.814949	-1.104071
1	-5.215167	0.426857	-0.489323
1	-6.898066	0.554706	0.091175
1	-5.564935	1.044101	1.149054
1	-6.111959	-0.506350	2.997840

1	-7.625392	-0.842413	2.115969
1	-6.596142	-2.182934	2.694201
1	1.540235	4.152987	5.456955
1	1.426476	2.575560	6.236451
1	-0.966005	2.156561	6.250181
1	-0.927337	3.921931	5.993993
1	-1.977805	2.904920	4.988866
1	-0.944743	3.645636	2.806587
1	-0.062901	4.848816	3.787151
1	0.811483	3.785600	2.644638
1	2.376268	0.250508	0.364306
6	-0.373255	2.664530	0.142328
6	-0.387893	4.053484	-0.012520
6	-1.599916	1.983978	0.262107
6	-1.596419	4.752114	-0.019410
1	0.556913	4.591841	-0.106907
6	-2.793014	2.689455	0.249133
1	-1.586592	0.898377	0.370233
6	-2.821430	4.088652	0.114845
1	-1.568349	5.834991	-0.136187
1	-3.726262	2.129523	0.339377
6	-4.171824	4.806979	0.106820
6	-4.019416	6.310533	-0.134763
1	-5.010791	6.786461	-0.145905

1	-3.425850	6.789470	0.657835
1	-3.535378	6.513839	-1.101787
6	-5.050830	4.217833	-1.010151
1	-5.249291	3.147699	-0.849037
1	-6.020346	4.738049	-1.044878
1	-4.562018	4.328138	-1.990156
6	-4.858786	4.590780	1.465493
1	-4.242965	4.996628	2.282090
1	-5.838004	5.093550	1.484445
1	-5.022535	3.521079	1.663319

Table S13

[P-TS]³

E : -3600.44991511 Hartree

G : -3598.909518 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
15	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.382000
6	1.132412	0.000000	2.887798
6	-1.724679	-0.608711	-0.095656

6	-2.038042	-1.982568	-0.027565
6	-2.819285	0.270239	-0.253825
6	-1.067587	-3.142660	0.134426
6	-3.354048	-2.448309	-0.124731
6	-2.763447	1.770542	-0.525835
6	-4.137468	-0.191392	-0.290879
6	-1.940566	-4.366112	-0.287393
6	-0.480424	-3.269020	1.539796
6	0.201606	-3.041649	-0.693494
6	-3.432285	-3.966872	-0.144065
6	-4.419466	-1.556399	-0.230439
6	-4.256317	2.205732	-0.417262
6	-2.127625	2.044381	-1.888418
6	-1.842168	2.563819	0.388870
6	-5.149727	0.933379	-0.420561
1	-1.682848	-5.265659	0.289695
1	-1.728322	-4.580400	-1.345551
6	0.910778	-3.466090	1.481634
6	-1.100312	-3.160647	2.768997
6	1.340503	-3.298155	0.084506
6	0.331976	-2.627752	-2.003657
6	-4.064229	-4.523540	1.138895
6	-4.244471	-4.455480	-1.349096
1	-5.450250	-1.918452	-0.288376

1	-4.521184	2.898116	-1.228918
1	-4.393947	2.751886	0.527106
6	-1.012460	2.887707	-1.765468
6	-2.505864	1.583913	-3.135236
6	-0.825689	3.199302	-0.339775
6	-1.892886	2.693295	1.764674
6	-5.972160	0.807329	-1.709074
6	-6.101451	0.933042	0.782923
6	1.634439	-3.650406	2.649934
6	-0.373346	-3.302310	3.967049
1	-2.163365	-2.914443	2.812704
6	2.599627	-3.200377	-0.491308
6	1.603583	-2.410208	-2.564324
1	-0.566380	-2.369960	-2.572151
1	-5.074397	-4.111505	1.284871
1	-4.147219	-5.619402	1.076446
1	-3.462860	-4.282936	2.024657
1	-5.305131	-4.177484	-1.252272
1	-4.190167	-5.552279	-1.427680
1	-3.859591	-4.020426	-2.283169
6	-0.296292	3.254535	-2.896058
6	-1.824331	1.987443	-4.299595
1	-3.351353	0.897648	-3.217865
6	0.156060	3.913247	0.328981

6	-0.907922	3.417914	2.460452
1	-2.700643	2.205366	2.316624
1	-6.530704	-0.140738	-1.727528
1	-6.697956	1.631668	-1.781620
1	-5.331328	0.841536	-2.600777
1	-6.711630	0.017168	0.804262
1	-6.783720	1.795893	0.735441
1	-5.536475	0.988337	1.725354
6	1.002335	-3.604768	3.905567
1	2.714377	-3.806522	2.596735
6	-1.131079	-3.103657	5.283865
6	2.748965	-2.757351	-1.818233
1	3.486605	-3.415912	0.109883
6	1.658203	-1.706879	-3.923935
6	-0.689137	2.817809	-4.173971
1	0.576489	3.901693	-2.790848
6	-2.370764	1.499335	-5.648373
6	0.137589	4.027524	1.729456
1	0.965264	4.373779	-0.240406
6	-1.044445	3.574144	3.979570
6	1.853673	-3.858744	5.154399
6	-0.152922	-3.041501	6.467217
6	-1.906500	-1.776766	5.253092
6	-2.123987	-4.260998	5.480975

6	4.163061	-2.613888	-2.386173
6	1.017990	-2.597251	-5.000477
6	3.106566	-1.371505	-4.322470
6	0.883002	-0.381872	-3.828318
6	0.110334	3.307232	-5.386553
6	-1.713680	2.263694	-6.808640
6	-2.112083	-0.008694	-5.806758
6	-3.886771	1.741751	-5.728553
6	1.314610	4.746612	2.399426
6	0.314694	3.941851	4.591116
6	-2.079991	4.679317	4.255594
6	-1.517409	2.284066	4.662859
6	0.942211	-4.088209	6.368968
6	2.719578	-5.114169	4.972012
6	2.778126	-2.656097	5.401972
1	-0.722144	-3.155936	7.403596
1	0.301588	-2.037968	6.501740
1	-1.229749	-0.943431	5.010753
1	-2.353823	-1.584896	6.240982
1	-2.722702	-1.784698	4.516128
1	-2.823267	-4.324833	4.633992
1	-2.712371	-4.108336	6.399198
1	-1.605987	-5.227919	5.555995
6	4.089205	-2.453001	-3.911742

6	4.842958	-1.393124	-1.743077
6	5.003267	-3.863365	-2.085650
1	-0.014857	-2.865202	-4.734008
1	0.992959	-2.067396	-5.965751
1	1.582804	-3.532005	-5.133440
1	3.399756	-0.418158	-3.854775
1	3.144089	-1.201036	-5.410182
1	1.289384	0.256474	-3.027708
1	0.965575	0.166348	-4.780856
1	-0.187538	-0.524847	-3.620014
6	-0.218823	2.445467	-6.614536
6	1.623529	3.217193	-5.138132
6	-0.249773	4.779251	-5.654887
1	-2.193517	3.250913	-6.907244
1	-1.921466	1.726103	-7.747685
1	-2.515918	-0.568970	-4.949359
1	-2.600892	-0.381415	-6.720372
1	-1.038856	-0.232630	-5.873252
1	-4.128575	2.790966	-5.503079
1	-4.243648	1.514677	-6.745164
1	-4.447942	1.102599	-5.032090
6	0.989516	5.088245	3.861102
6	1.659222	6.059225	1.681196
6	2.534281	3.809769	2.338525

1	0.171168	4.190476	5.655038
1	0.961726	3.048485	4.559951
1	-3.060343	4.391144	3.847746
1	-2.191001	4.840610	5.339679
1	-1.797113	5.631668	3.786018
1	-0.830986	1.454457	4.443468
1	-1.534693	2.436893	5.753114
1	-2.533327	1.990263	4.362338
1	1.560002	-4.092730	7.281296
1	0.490396	-5.091653	6.292049
1	2.103401	-5.980001	4.687811
1	3.231360	-5.349385	5.918130
1	3.493768	-4.976059	4.204198
1	3.427510	-2.471286	4.531738
1	3.419669	-2.841445	6.278677
1	2.205904	-1.734187	5.575174
1	5.097057	-2.230750	-4.297684
1	3.787099	-3.418097	-4.353625
1	4.922824	-1.529290	-0.654422
1	5.858273	-1.255752	-2.147842
1	4.269722	-0.470276	-1.908224
1	4.499515	-4.771282	-2.448502
1	5.978121	-3.783585	-2.590984
1	5.198575	-3.986443	-1.011074

1	0.234303	2.908602	-7.505724
1	0.263021	1.459621	-6.497869
1	1.914365	2.205749	-4.819668
1	2.162638	3.455646	-6.067944
1	1.963374	3.928124	-4.372399
1	0.002557	5.399615	-4.782366
1	0.311870	5.160085	-6.522542
1	-1.323604	4.908520	-5.849061
1	1.923524	5.375167	4.370504
1	0.338663	5.977539	3.888086
1	0.772876	6.705099	1.593853
1	2.425233	6.601450	2.256864
1	2.065388	5.893218	0.673975
1	2.783551	3.565264	1.295401
1	3.411904	4.288075	2.801974
1	2.339346	2.858689	2.853376
1	-1.076600	-0.064402	2.482239
6	2.546724	-0.076880	3.073234
6	3.198430	0.543834	4.146765
6	3.315431	-0.829246	2.164655
6	4.571816	0.392889	4.326896
1	2.614697	1.128471	4.860260
6	4.680492	-0.975852	2.360758
1	2.818225	-1.299251	1.313816

6	5.340866	-0.380184	3.448973
1	5.038316	0.881986	5.181195
1	5.249585	-1.579207	1.649553
6	6.842137	-0.610433	3.635328
6	7.388464	0.132216	4.857463
1	8.467927	-0.055656	4.951331
1	7.242185	1.218803	4.768081
1	6.906253	-0.208024	5.785707
6	7.093251	-2.115949	3.826540
1	6.760882	-2.694660	2.952571
1	8.167459	-2.308297	3.971269
1	6.551188	-2.491083	4.707673
6	7.593422	-0.116782	2.387873
1	7.421403	0.958197	2.230595
1	8.675297	-0.281387	2.506758
1	7.269293	-0.647364	1.481100

Table S14

[As-TS]³

E : -5494.85780557 Hartree

G : -5493.318336 Hartree

Atomic

Coordinates (Angstroms)

Number	X	Y	Z
33	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.396902
6	1.125727	0.000000	2.934018
6	-1.848397	-0.661011	-0.057237
6	-2.150029	-2.031056	0.062364
6	-2.945820	0.207792	-0.226870
6	-1.176384	-3.187764	0.246352
6	-3.467549	-2.505237	0.008275
6	-2.909583	1.698744	-0.557604
6	-4.264002	-0.259874	-0.221554
6	-2.056050	-4.424540	-0.119905
6	-0.567006	-3.273486	1.645428
6	0.079153	-3.127092	-0.605741
6	-3.543886	-4.023258	0.045014
6	-4.538099	-1.622153	-0.107033
6	-4.400786	2.129923	-0.420534
6	-2.316409	1.922459	-1.948008
6	-1.969328	2.533560	0.296942
6	-5.285984	0.853841	-0.368181
1	-1.782756	-5.306687	0.476577
1	-1.867390	-4.668339	-1.176158
6	0.819803	-3.494286	1.570050

6	-1.162769	-3.115573	2.881394
6	1.227655	-3.374604	0.161331
6	0.192740	-2.762408	-1.932215
6	-4.143383	-4.534512	1.362004
6	-4.383792	-4.556228	-1.121565
1	-5.568190	-1.990169	-0.130788
1	-4.691177	2.802062	-1.240448
1	-4.515137	2.696965	0.514638
6	-1.212677	2.788096	-1.892850
6	-2.712632	1.392105	-3.161104
6	-0.985472	3.154406	-0.485903
6	-1.967516	2.694680	1.671010
6	-6.131703	0.683316	-1.636417
6	-6.215681	0.885885	0.852045
6	1.560975	-3.655979	2.730862
6	-0.416824	-3.232144	4.070528
1	-2.220771	-2.850085	2.936013
6	2.478253	-3.308082	-0.436909
6	1.457376	-2.582185	-2.521869
1	-0.712054	-2.515630	-2.495424
1	-5.150241	-4.118056	1.517944
1	-4.226322	-5.631955	1.340274
1	-3.520682	-4.262463	2.223475
1	-5.442679	-4.277653	-1.008473

1	-4.327853	-5.655004	-1.162449
1	-4.023493	-4.153720	-2.079739
6	-0.527541	3.108426	-3.056490
6	-2.063170	1.746220	-4.359267
1	-3.544599	0.685264	-3.189431
6	0.028658	3.873333	0.128374
6	-0.950743	3.425088	2.310722
1	-2.752114	2.218181	2.264111
1	-6.680007	-0.270707	-1.617448
1	-6.867843	1.497680	-1.717147
1	-5.509140	0.700205	-2.541292
1	-6.821725	-0.031037	0.911642
1	-6.902244	1.744504	0.791317
1	-5.633935	0.971116	1.781936
6	0.952140	-3.561208	3.995107
1	2.636951	-3.832721	2.663943
6	-1.147657	-2.976892	5.392948
6	2.610994	-2.911530	-1.780192
1	3.372275	-3.512068	0.157539
6	1.496343	-1.943854	-3.914295
6	-0.940238	2.600619	-4.301563
1	0.338076	3.771410	-3.003569
6	-2.627950	1.178074	-5.668546
6	0.075632	4.002289	1.526283

1	0.821237	4.309957	-0.481870
6	-1.022975	3.628811	3.828003
6	1.819280	-3.794053	5.237252
6	-0.150438	-2.907997	6.560080
6	-1.887055	-1.630544	5.335759
6	-2.167363	-4.101263	5.638099
6	4.017105	-2.792639	-2.372425
6	0.822806	-2.876877	-4.933118
6	2.940793	-1.650101	-4.359067
6	0.742560	-0.603619	-3.870185
6	-0.174224	3.037965	-5.554856
6	-2.009507	1.892268	-6.880713
6	-2.342652	-0.331032	-5.753198
6	-4.149647	1.388199	-5.728343
6	1.312700	4.673585	2.135427
6	0.381464	3.915876	4.376479
6	-1.969298	4.811799	4.103222
6	-1.561000	2.398065	4.568736
6	0.921908	-3.978609	6.469820
6	2.664118	-5.066571	5.075841
6	2.764905	-2.599309	5.440427
1	-0.707686	-2.989502	7.507028
1	0.324902	-1.913664	6.565224
1	-1.189023	-0.823090	5.067577

1	-2.319651	-1.401870	6.322398
1	-2.709701	-1.633668	4.605852
1	-2.881534	-4.171486	4.804180
1	-2.737048	-3.906493	6.560097
1	-1.673178	-5.078800	5.734115
6	3.921533	-2.715037	-3.903265
6	4.694921	-1.534278	-1.803301
6	4.871043	-4.018037	-2.017102
1	-0.207914	-3.117593	-4.634486
1	0.785918	-2.394935	-5.922748
1	1.373532	-3.824427	-5.029984
1	3.253487	-0.673661	-3.956587
1	2.958852	-1.546079	-5.455573
1	1.182854	0.069492	-3.117497
1	0.807288	-0.108405	-4.852807
1	-0.323781	-0.717508	-3.625012
6	-0.514288	2.107795	-6.728719
6	1.344884	2.983227	-5.334188
6	-0.563295	4.488226	-5.892152
1	-2.508574	2.865110	-7.018798
1	-2.227742	1.303622	-7.786163
1	-2.716728	-0.852809	-4.858749
1	-2.842832	-0.761051	-6.634929
1	-1.266637	-0.536841	-5.831785

1	-4.407043	2.443186	-5.552506
1	-4.522999	1.101762	-6.723813
1	-4.683827	0.776194	-4.987678
6	1.085807	5.023467	3.614346
6	1.677929	5.970375	1.399732
6	2.482116	3.679364	2.010788
1	0.302103	4.172780	5.445210
1	0.970902	2.984656	4.315687
1	-2.983300	4.574437	3.748349
1	-2.020972	5.020168	5.183837
1	-1.646803	5.725023	3.584293
1	-0.945687	1.513977	4.352410
1	-1.523207	2.584115	5.653158
1	-2.607197	2.173299	4.317131
1	1.552954	-3.975257	7.373018
1	0.449338	-4.974324	6.421543
1	2.031330	-5.930473	4.824084
1	3.186646	-5.284027	6.020316
1	3.428756	-4.960447	4.293529
1	3.410821	-2.452674	4.560436
1	3.409911	-2.768352	6.317826
1	2.209550	-1.662775	5.588438
1	4.924738	-2.521008	-4.315666
1	3.606884	-3.701090	-4.286379

1	4.791210	-1.613212	-0.710231
1	5.702878	-1.408675	-2.229873
1	4.110229	-0.626308	-2.006689
1	4.368483	-4.948256	-2.320254
1	5.836651	-3.959831	-2.542590
1	5.086225	-4.079843	-0.941067
1	-0.087398	2.530299	-7.652411
1	-0.013929	1.137128	-6.570418
1	1.657438	1.993965	-4.969908
1	1.861228	3.180439	-6.286301
1	1.689239	3.737986	-4.613749
1	-0.303389	5.157597	-5.058966
1	-0.025480	4.831014	-6.790222
1	-1.642710	4.591086	-6.070442
1	2.061546	5.248877	4.074000
1	0.494246	5.950991	3.681206
1	0.818793	6.656587	1.360773
1	2.498027	6.475547	1.933003
1	2.020931	5.788620	0.371933
1	2.666606	3.427641	0.955894
1	3.403941	4.112222	2.431036
1	2.266288	2.736762	2.533636
1	-1.072177	-0.081010	2.542854
6	2.544855	-0.083283	3.069975

6	3.245716	0.577122	4.088365
6	3.271717	-0.884557	2.167343
6	4.623306	0.417757	4.221473
1	2.696900	1.200191	4.796982
6	4.641922	-1.037895	2.316048
1	2.738365	-1.387604	1.358600
6	5.350366	-0.402506	3.350102
1	5.127990	0.938832	5.034183
1	5.176248	-1.678689	1.610396
6	6.855549	-0.640876	3.488088
6	7.455869	0.147526	4.654970
1	8.536360	-0.048024	4.715586
1	7.316288	1.230797	4.524191
1	7.006499	-0.147113	5.614753
6	7.100666	-2.139397	3.734121
1	6.729435	-2.751286	2.899266
1	8.177927	-2.336783	3.845640
1	6.589826	-2.470866	4.650687
6	7.561808	-0.209232	2.192259
1	7.394435	0.860062	1.996037
1	8.645862	-0.381369	2.275410
1	7.196323	-0.773886	1.322508

Table S15**[Sb-TS]³**

E : -3499.42298532 Hartree

G : -3497.885789 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
51	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.478751
6	1.121452	0.000000	3.046891
6	-2.058178	-0.771780	0.037330
6	-2.325385	-2.141318	0.212378
6	-3.179939	0.067301	-0.109397
6	-1.327253	-3.278055	0.412043
6	-3.635083	-2.645437	0.230988
6	-3.198585	1.553780	-0.473145
6	-4.488293	-0.427051	-0.038962
6	-2.196070	-4.542617	0.122053
6	-0.682598	-3.302541	1.798058
6	-0.093912	-3.254439	-0.473306
6	-3.682633	-4.161457	0.329441
6	-4.727525	-1.789695	0.128856
6	-4.694273	1.950912	-0.288045

6	-2.662941	1.766499	-1.887316
6	-2.257773	2.437382	0.329087
6	-5.543475	0.655192	-0.182818
1	-1.882962	-5.398752	0.736713
1	-2.042826	-4.818749	-0.932008
6	0.700252	-3.537158	1.697872
6	-1.244962	-3.088047	3.041519
6	1.072584	-3.476850	0.275445
6	-0.010827	-2.958995	-1.819827
6	-4.220956	-4.631355	1.687758
6	-4.556567	-4.754838	-0.781737
1	-5.749490	-2.179627	0.158182
1	-5.031800	2.603518	-1.105769
1	-4.788010	2.528691	0.642821
6	-1.594997	2.678387	-1.891627
6	-3.069891	1.180738	-3.070948
6	-1.334753	3.087652	-0.501841
6	-2.201976	2.612795	1.701108
6	-6.415234	0.432597	-1.425348
6	-6.443938	0.693182	1.058784
6	1.469033	-3.663118	2.845434
6	-0.470373	-3.166861	4.215420
1	-2.298969	-2.810018	3.111036
6	2.308153	-3.443216	-0.354873

6	1.240089	-2.820871	-2.450608
1	-0.928624	-2.739017	-2.373106
1	-5.227936	-4.225073	1.867967
1	-4.285790	-5.730040	1.710345
1	-3.569498	-4.317077	2.512832
1	-5.615465	-4.491045	-0.637705
1	-4.481010	-5.853249	-0.782490
1	-4.241628	-4.383726	-1.768171
6	-0.947776	2.977792	-3.082134
6	-2.464148	1.516083	-4.297012
1	-3.873685	0.441646	-3.052732
6	-0.318295	3.846277	0.061486
6	-1.184067	3.382783	2.288976
1	-2.941584	2.113440	2.331727
1	-6.934011	-0.536528	-1.372350
1	-7.177043	1.223259	-1.504417
1	-5.816152	0.448142	-2.345978
1	-7.027197	-0.235530	1.152961
1	-7.151713	1.534309	0.996323
1	-5.842406	0.812094	1.972230
6	0.892837	-3.515104	4.119646
1	2.541001	-3.855306	2.759091
6	-1.165479	-2.851828	5.544414
6	2.410029	-3.114802	-1.719192

1	3.215305	-3.622760	0.227095
6	1.248839	-2.279384	-3.884858
6	-1.367510	2.405707	-4.296821
1	-0.103057	3.669434	-3.074596
6	-3.050636	0.896861	-5.572923
6	-0.208308	3.980508	1.454840
1	0.433866	4.299490	-0.586589
6	-1.202087	3.610841	3.804526
6	1.785503	-3.716413	5.349453
6	-0.141367	-2.762958	6.686675
6	-1.878086	-1.493015	5.456420
6	-2.200975	-3.946246	5.850956
6	3.802920	-3.029193	-2.347078
6	0.551910	-3.282806	-4.817887
6	2.682980	-2.021172	-4.382120
6	0.497386	-0.937476	-3.926911
6	-0.627700	2.802683	-5.578806
6	-2.480306	1.591282	-6.819376
6	-2.736707	-0.607795	-5.625061
6	-4.577519	1.074937	-5.594512
6	1.050056	4.659473	2.009317
6	0.215849	3.930450	4.297821
6	-2.155935	4.785453	4.091090
6	-1.695046	2.387210	4.586111

6	0.912393	-3.852340	6.605495
6	2.612540	-5.003316	5.211440
6	2.748717	-2.526964	5.495593
1	-0.678293	-2.806453	7.647740
1	0.349417	-1.776860	6.650258
1	-1.165246	-0.709516	5.158227
1	-2.293801	-1.226378	6.440849
1	-2.708850	-1.499384	4.735577
1	-2.935950	-4.030944	5.036718
1	-2.745052	-3.708358	6.778243
1	-1.723444	-4.929564	5.970090
6	3.674823	-3.052972	-3.877216
6	4.483427	-1.732855	-1.874075
6	4.673199	-4.223810	-1.931435
1	-0.470820	-3.500622	-4.477277
1	0.490568	-2.873426	-5.838348
1	1.101046	-4.235261	-4.858717
1	3.005809	-1.019747	-4.056490
1	2.675119	-1.993911	-5.483292
1	0.959298	-0.208008	-3.242834
1	0.539898	-0.522209	-4.947449
1	-0.562275	-1.029619	-3.645974
6	-0.985040	1.831682	-6.713832
6	0.894564	2.751064	-5.379723

6	-1.022413	4.239875	-5.960355
1	-2.998290	2.553365	-6.964177
1	-2.715286	0.978399	-7.704280
1	-3.073892	-1.112275	-4.706450
1	-3.253205	-1.071763	-6.479714
1	-1.659398	-0.793777	-5.730296
1	-4.851549	2.129357	-5.442244
1	-4.973374	0.751411	-6.569727
1	-5.076992	0.475130	-4.820399
6	0.876120	5.032380	3.489047
6	1.397554	5.941948	1.241557
6	2.208241	3.654220	1.860019
1	0.167761	4.210604	5.362565
1	0.817695	3.007047	4.239395
1	-3.178175	4.527066	3.776893
1	-2.172278	5.013162	5.168897
1	-1.865267	5.693252	3.544532
1	-1.076280	1.508012	4.361227
1	-1.617085	2.592073	5.664938
1	-2.747136	2.145046	4.379395
1	1.562696	-3.832879	7.494687
1	0.424278	-4.841726	6.595493
1	1.964504	-5.867703	5.003980
1	3.154894	-5.194974	6.150293

1	3.359622	-4.932669	4.408508
1	3.388670	-2.425658	4.605061
1	3.399490	-2.670220	6.373190
1	2.207736	-1.577229	5.609964
1	4.668463	-2.885249	-4.322932
1	3.355048	-4.062715	-4.187390
1	4.598006	-1.738651	-0.779731
1	5.483251	-1.631306	-2.325539
1	3.890506	-0.842892	-2.127230
1	4.169085	-5.175047	-2.156810
1	5.624089	-4.197090	-2.485393
1	4.918043	-4.210721	-0.860080
1	-0.586543	2.229254	-7.660924
1	-0.468459	0.873096	-6.536101
1	1.207706	1.770218	-4.993367
1	1.397569	2.919934	-6.344419
1	1.251595	3.523455	-4.684561
1	-0.754601	4.938582	-5.154207
1	-0.495321	4.552241	-6.875613
1	-2.103924	4.334709	-6.130617
1	1.866439	5.276308	3.906145
1	0.276937	5.954563	3.562320
1	0.541917	6.633311	1.220930
1	2.238355	6.449797	1.738634

1	1.704955	5.742286	0.205858
1	2.363941	3.398810	0.801057
1	3.144404	4.079974	2.255313
1	1.996767	2.714785	2.391540
1	-1.062118	-0.110059	2.687028
6	2.546240	-0.070786	3.095231
6	3.308864	0.658179	4.019681
6	3.221420	-0.929224	2.202777
6	4.692843	0.511823	4.072568
1	2.802451	1.326505	4.718691
6	4.599751	-1.066718	2.270314
1	2.643250	-1.491215	1.467011
6	5.369223	-0.361748	3.211245
1	5.245404	1.087755	4.814079
1	5.091414	-1.751483	1.574819
6	6.882405	-0.583172	3.264363
6	7.550881	0.282250	4.335751
1	8.634708	0.095855	4.337698
1	7.393761	1.354080	4.144564
1	7.167825	0.048982	5.340120
6	7.158360	-2.061209	3.588813
1	6.739375	-2.727593	2.821020
1	8.242575	-2.244718	3.641293
1	6.711925	-2.336127	4.556239

6	7.497967	-0.232344	1.899580
1	7.307515	0.821025	1.646552
1	8.586822	-0.392681	1.921677
1	7.081789	-0.854136	1.093867

Table S16

[Bi-TS]³

E : -3473.75910665 Hartree

G : -3472.221471 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
83	0.010312	0.004584	-0.033495
6	0.004589	0.045099	2.399506
6	1.116762	0.068751	3.014753
6	-2.161895	-0.775213	0.024147
6	-2.442685	-2.126631	0.280113
6	-3.270521	0.067076	-0.169196
6	-1.456203	-3.266248	0.522988
6	-3.759070	-2.613018	0.334660
6	-3.272465	1.529383	-0.623489
6	-4.585748	-0.403401	-0.060255

6	-2.346009	-4.531455	0.305849
6	-0.782850	-3.243569	1.895649
6	-0.240849	-3.298541	-0.386094
6	-3.823855	-4.120429	0.518103
6	-4.841205	-1.750306	0.190017
6	-4.760786	1.958693	-0.451634
6	-2.749152	1.650418	-2.053018
6	-2.308389	2.441299	0.116074
6	-5.626806	0.684084	-0.257157
1	-2.034599	-5.362796	0.954542
1	-2.214194	-4.857843	-0.736737
6	0.591658	-3.516676	1.777599
6	-1.312137	-2.961972	3.140553
6	0.936581	-3.517811	0.346715
6	-0.179628	-3.044594	-1.741937
6	-4.341536	-4.505862	1.910642
6	-4.725450	-4.764863	-0.541085
1	-5.867876	-2.124272	0.249083
1	-5.096813	2.561203	-1.307565
1	-4.838818	2.597205	0.440206
6	-1.668530	2.544692	-2.121772
6	-3.180976	1.008542	-3.198425
6	-1.383954	3.026366	-0.760262
6	-2.223342	2.680924	1.477179

6	-6.518876	0.400200	-1.472415
6	-6.509414	0.811536	0.991393
6	1.382001	-3.614756	2.913461
6	-0.513433	-3.006294	4.300145
1	-2.357135	-2.653171	3.219254
6	2.159503	-3.526291	-0.308857
6	1.060867	-2.946949	-2.400913
1	-1.104710	-2.824791	-2.282795
1	-5.340845	-4.078563	2.084784
1	-4.416775	-5.600651	1.998170
1	-3.672207	-4.151457	2.704497
1	-5.778520	-4.481482	-0.391755
1	-4.661431	-5.862428	-0.481782
1	-4.426407	-4.452946	-1.552633
6	-1.035027	2.771760	-3.335740
6	-2.588767	1.269450	-4.449163
1	-3.995487	0.284301	-3.129777
6	-0.336687	3.782536	-0.251773
6	-1.173626	3.448673	2.008803
1	-2.959436	2.226405	2.144107
1	-7.057646	-0.551544	-1.349643
1	-7.264474	1.200694	-1.595265
1	-5.931305	0.341047	-2.398825
1	-7.101021	-0.102589	1.152344

1	-7.208926	1.655231	0.884965
1	-5.893624	0.981259	1.887106
6	0.838330	-3.393072	4.190684
1	2.446332	-3.838737	2.813590
6	-1.171965	-2.602397	5.624767
6	2.240065	-3.241914	-1.685010
1	3.075486	-3.703007	0.260328
6	1.051410	-2.445886	-3.849263
6	-1.481320	2.143389	-4.512509
1	-0.183019	3.453256	-3.377053
6	-3.201651	0.590052	-5.681455
6	-0.194259	3.974598	1.131576
1	0.418430	4.178543	-0.933580
6	-1.143818	3.746559	3.510605
6	1.747520	-3.547526	5.413852
6	-0.146531	-2.562668	6.771629
6	-1.773898	-1.194278	5.491813
6	-2.286519	-3.604284	5.968588
6	3.623096	-3.207947	-2.340009
6	0.350298	-3.477797	-4.747203
6	2.480476	-2.192647	-4.359747
6	0.293367	-1.109390	-3.924797
6	-0.761254	2.467518	-5.826032
6	-2.641391	1.207097	-6.972541

6	-2.908095	-0.919419	-5.655417
6	-4.726342	0.787363	-5.691557
6	1.105838	4.621233	1.628210
6	0.308893	3.963584	3.955178
6	-1.988447	5.010809	3.756145
6	-1.723665	2.608015	4.357587
6	0.879615	-3.676518	6.673574
6	2.605925	-4.815773	5.304300
6	2.681152	-2.330139	5.522758
1	-0.688410	-2.614799	7.729399
1	0.370007	-1.589833	6.763904
1	-0.997018	-0.480268	5.178053
1	-2.175488	-0.865979	6.463552
1	-2.595191	-1.156726	4.760495
1	-3.022837	-3.677348	5.154876
1	-2.816450	-3.286045	6.879627
1	-1.877633	-4.611204	6.138875
6	3.471227	-3.232078	-3.868353
6	4.360859	-1.936771	-1.885459
6	4.453813	-4.433619	-1.932848
1	-0.671590	-3.680683	-4.394609
1	0.285593	-3.102190	-5.780498
1	0.895505	-4.433074	-4.758685
1	2.809937	-1.194784	-4.028803

1	2.462497	-2.157160	-5.460620
1	0.761426	-0.356398	-3.270435
1	0.324763	-0.723609	-4.956922
1	-0.763946	-1.194548	-3.633693
6	-1.142799	1.439613	-6.901568
6	0.764280	2.421479	-5.652287
6	-1.157556	3.884555	-6.275896
1	-3.152842	2.164060	-7.165817
1	-2.893573	0.547145	-7.817969
1	-3.237735	-1.368212	-4.705700
1	-3.443853	-1.422268	-6.475470
1	-1.835125	-1.126280	-5.766360
1	-4.984595	1.852213	-5.594103
1	-5.140548	0.415989	-6.641767
1	-5.222070	0.238107	-4.878539
6	1.018098	5.009088	3.112929
6	1.456304	5.885582	0.832301
6	2.224886	3.578301	1.440223
1	0.318497	4.256093	5.017685
1	0.835881	2.995937	3.885257
1	-3.039959	4.816544	3.497279
1	-1.941524	5.304945	4.816952
1	-1.651786	5.856893	3.141447
1	-1.201936	1.663574	4.151646

1	-1.590033	2.846035	5.423950
1	-2.800618	2.463519	4.192001
1	1.534017	-3.682056	7.560001
1	0.367709	-4.654093	6.652360
1	1.979322	-5.702699	5.128226
1	3.161247	-4.965735	6.243041
1	3.345348	-4.749408	4.494139
1	3.354072	-2.275646	4.652575
1	3.298905	-2.402425	6.432546
1	2.119631	-1.385805	5.550148
1	4.459659	-3.073096	-4.328519
1	3.139442	-4.239177	-4.173842
1	4.470430	-1.927071	-0.790780
1	5.366075	-1.889579	-2.333632
1	3.811079	-1.025106	-2.159067
1	3.909279	-5.365198	-2.145758
1	5.395959	-4.446203	-2.502124
1	4.715134	-4.425669	-0.865362
1	-0.755867	1.782357	-7.874559
1	-0.630656	0.487426	-6.680968
1	1.083751	1.462004	-5.220214
1	1.249618	2.537386	-6.633657
1	1.135859	3.229043	-5.006466
1	-0.871017	4.623306	-5.513028

1	-0.647253	4.145487	-7.216434
1	-2.241784	3.975992	-6.429641
1	2.040421	5.176859	3.488391
1	0.496619	5.975092	3.208107
1	0.625323	6.606394	0.853578
1	2.340528	6.366539	1.278306
1	1.697234	5.668817	-0.217604
1	2.313164	3.288756	0.382082
1	3.193864	3.985719	1.769908
1	2.017449	2.662687	2.014375
1	-1.037884	-0.080982	2.696575
6	2.542655	0.002029	3.008196
6	3.341807	0.799100	3.843467
6	3.187966	-0.927454	2.163718
6	4.727139	0.658233	3.851600
1	2.861883	1.520086	4.508128
6	4.568066	-1.059833	2.187629
1	2.583450	-1.548963	1.500649
6	5.372857	-0.280181	3.035706
1	5.306675	1.291841	4.522195
1	5.033751	-1.799072	1.530982
6	6.888106	-0.493683	3.042828
6	7.596689	0.460266	4.008039
1	8.680937	0.278669	3.977394

1	7.423264	1.511852	3.735712
1	7.259904	0.310131	5.044338
6	7.186451	-1.938629	3.477800
1	6.738620	-2.667874	2.787302
1	8.272990	-2.114877	3.498618
1	6.783418	-2.132422	4.483123
6	7.443852	-0.257797	1.628555
1	7.238526	0.770674	1.296835
1	8.533329	-0.415201	1.617326
1	6.996282	-0.944985	0.896090

Table S17

[N-Int]³

E : -3313.93388839 Hartree

G : -3312.380112 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
7	0.501880	-0.514091	-0.056431
6	1.359706	0.437217	0.141221
6	0.981537	1.797205	0.141868
6	0.950923	-1.837524	-0.117714

6	1.651836	-2.337802	-1.226784
6	0.626197	-2.748328	0.898369
6	2.055077	-1.561508	-2.468532
6	2.022930	-3.682369	-1.303940
6	-0.249520	-2.476062	2.107884
6	1.068257	-4.070416	0.856910
6	2.445522	-2.705118	-3.455642
6	3.152852	-0.538161	-2.179158
6	0.952193	-0.653260	-2.997537
6	2.682081	-4.006154	-2.636579
6	1.764510	-4.559901	-0.250426
6	0.003032	-3.736092	2.992480
6	-1.710671	-2.274884	1.703529
6	0.042879	-1.152811	2.800045
6	0.706847	-4.824792	2.127026
1	3.317163	-2.429898	-4.066462
1	1.601098	-2.861354	-4.143138
6	2.760738	0.744326	-2.592246
6	4.319039	-0.694175	-1.450928
6	1.403051	0.665207	-3.146509
6	-0.386411	-0.944387	-3.172980
6	4.174458	-4.319128	-2.463570
6	1.997315	-5.202349	-3.307579
1	2.084606	-5.604676	-0.296763

1	-0.935303	-4.102128	3.432998
1	0.659937	-3.448542	3.826410
6	-2.184992	-1.024217	2.129713
6	-2.561172	-3.136565	1.037679
6	-1.084530	-0.318753	2.802785
6	1.244693	-0.688383	3.297556
6	-0.204808	-6.023780	1.839135
6	1.980515	-5.324955	2.821817
6	3.520549	1.850234	-2.237455
6	5.102018	0.414677	-1.080638
1	4.591315	-1.685237	-1.087797
6	0.537322	1.649170	-3.600931
6	-1.300638	0.066778	-3.519028
1	-0.746983	-1.953441	-2.953701
1	4.315640	-5.174363	-1.785488
1	4.627049	-4.572542	-3.434533
1	4.722820	-3.462578	-2.049596
1	2.156863	-6.125605	-2.730014
1	2.404831	-5.361443	-4.317966
1	0.913554	-5.034334	-3.392137
6	-3.493424	-0.648820	1.856138
6	-3.910711	-2.802686	0.810585
1	-2.182882	-4.099741	0.689805
6	-0.999605	0.959112	3.334011

6	1.361166	0.622535	3.797557
1	2.125254	-1.335085	3.254133
1	0.290110	-6.735906	1.161649
1	-0.447820	-6.553982	2.772668
1	-1.148287	-5.712527	1.371040
1	2.501738	-6.069933	2.201543
1	1.734007	-5.795889	3.786147
1	2.673969	-4.491608	3.008748
6	4.685038	1.709448	-1.466223
1	3.162256	2.847673	-2.500984
6	6.389855	0.169241	-0.288917
6	-0.818079	1.356985	-3.826622
1	0.903812	2.667531	-3.752141
6	-2.793588	-0.261515	-3.438793
6	-4.372688	-1.525228	1.193798
1	-3.845638	0.335018	2.176449
6	-4.812544	-3.876275	0.184945
6	0.213433	1.444740	3.850835
1	-1.880404	1.605407	3.324014
6	2.741176	1.102482	4.256861
6	5.369908	2.987108	-0.968120
6	6.788864	1.443017	0.470223
6	6.222272	-0.955521	0.742160
6	7.496162	-0.239094	-1.277993

6	-1.714022	2.467611	-4.383817
6	-3.182576	-1.269270	-4.530924
6	-3.624573	1.024376	-3.569342
6	-3.101473	-0.871377	-2.062320
6	-5.814333	-1.064264	0.951333
6	-6.289601	-3.461090	0.275421
6	-4.427362	-4.113938	-1.284599
6	-4.653847	-5.202911	0.946412
6	0.224610	2.868910	4.418574
6	2.749210	2.632616	4.380223
6	3.086859	0.447665	5.604689
6	3.819977	0.714373	3.234499
6	6.768047	2.678815	-0.412180
6	5.527783	4.018903	-2.093594
6	4.486550	3.591779	0.140291
1	7.790653	1.298141	0.905737
1	6.095861	1.577071	1.318048
1	5.342223	-0.777730	1.377168
1	7.112202	-0.995443	1.388748
1	6.115932	-1.944076	0.274040
1	7.210555	-1.160675	-1.806854
1	8.440583	-0.425770	-0.742566
1	7.671225	0.534742	-2.038254
6	-3.116396	1.917742	-4.686847

6	-1.809871	3.614765	-3.368608
6	-1.118499	3.006770	-5.693115
1	-2.584076	-2.188168	-4.444000
1	-4.244842	-1.545024	-4.435307
1	-3.019213	-0.860654	-5.538612
1	-3.579204	1.573521	-2.612099
1	-4.681219	0.753041	-3.726318
1	-2.770500	-0.203821	-1.252067
1	-4.188478	-1.020764	-1.959573
1	-2.616538	-1.845340	-1.906788
6	-6.501452	-1.995465	-0.058538
6	-5.853134	0.360659	0.377648
6	-6.576163	-1.069623	2.287949
1	-6.658835	-3.661834	1.294239
1	-6.879404	-4.103596	-0.397693
1	-3.354480	-4.340625	-1.378985
1	-4.993967	-4.967497	-1.688009
1	-4.637107	-3.234960	-1.908636
1	-4.809506	-5.056395	2.025485
1	-5.398593	-5.928481	0.583866
1	-3.659760	-5.649039	0.800775
6	1.546960	3.153071	5.146928
6	-0.919382	3.056529	5.426467
6	0.035219	3.867900	3.267034

1	3.688096	2.946585	4.864079
1	2.758207	3.066312	3.365163
1	3.088613	-0.648253	5.509275
1	4.086282	0.765342	5.941505
1	2.356524	0.708562	6.383192
1	3.545147	1.059070	2.224245
1	4.779049	1.181569	3.510541
1	3.983980	-0.371485	3.194290
1	7.126440	3.558085	0.146924
1	7.466891	2.543722	-1.253792
1	6.049237	3.580766	-2.957347
1	6.120093	4.872649	-1.729839
1	4.562179	4.413215	-2.438971
1	3.473355	3.795023	-0.240143
1	4.917880	4.536923	0.506151
1	4.382027	2.903706	0.992531
1	-3.800803	2.763928	-4.859352
1	-3.084234	1.345198	-5.629029
1	-0.817200	4.032560	-3.145452
1	-2.440235	4.427854	-3.764860
1	-2.234303	3.269460	-2.416344
1	-0.970361	2.194351	-6.419756
1	-1.802664	3.747487	-6.136191
1	-0.149593	3.499845	-5.530176

1	-7.576095	-1.754484	-0.090457
1	-6.105091	-1.784209	-1.066414
1	-5.214936	0.445181	-0.515534
1	-6.884601	0.617308	0.090461
1	-5.524511	1.110282	1.112460
1	-6.093088	-0.392646	3.007788
1	-7.613926	-0.731373	2.140244
1	-6.596093	-2.070188	2.741712
1	1.631447	4.238547	5.315261
1	1.517541	2.687107	6.145553
1	-0.880536	2.287842	6.212448
1	-0.831717	4.044745	5.904329
1	-1.906843	3.007386	4.946397
1	-0.893466	3.660431	2.712982
1	-0.016347	4.897250	3.656569
1	0.861309	3.807511	2.543380
1	2.430666	0.221832	0.298176
6	-0.239063	2.521327	0.048695
6	-0.257862	3.923329	-0.075639
6	-1.478346	1.845345	0.156631
6	-1.458079	4.626947	-0.050978
1	0.688806	4.460305	-0.166692
6	-2.662876	2.561890	0.183369
1	-1.476175	0.758130	0.236725

6	-2.686198	3.965798	0.091771
1	-1.425891	5.712069	-0.142582
1	-3.598194	2.005425	0.275080
6	-4.028885	4.694407	0.150377
6	-3.873373	6.201407	-0.067276
1	-4.860731	6.684432	-0.033129
1	-3.248155	6.660786	0.712387
1	-3.422929	6.420034	-1.047159
6	-4.962965	4.136507	-0.937334
1	-5.162258	3.064503	-0.792171
1	-5.929031	4.663568	-0.913108
1	-4.521472	4.268068	-1.936883
6	-4.656080	4.455565	1.534471
1	-4.001496	4.841847	2.330315
1	-5.630365	4.962963	1.607586
1	-4.816354	3.382686	1.718114

Table S18

[P-Int]³

E : -3600.47984284 Hartree

G : -3598.936658 Hartree

Atomic

Coordinates (Angstroms)

Number	X	Y	Z
15	-0.195534	-0.414044	-0.369838
6	1.007818	0.753705	0.257884
6	0.708439	2.055192	0.352288
6	0.742152	-1.997283	-0.200550
6	1.584835	-2.490455	-1.213046
6	0.516291	-2.836963	0.905318
6	2.100417	-1.745002	-2.447150
6	2.114713	-3.783997	-1.159024
6	-0.313402	-2.522732	2.151751
6	1.076492	-4.116097	0.976802
6	2.729753	-2.881976	-3.301964
6	3.069697	-0.636890	-2.031599
6	1.024299	-0.935011	-3.154873
6	2.904562	-4.143384	-2.406840
6	1.863657	-4.608501	-0.063710
6	-0.039522	-3.756038	3.072592
6	-1.793143	-2.274401	1.861230
6	0.069876	-1.207034	2.823057
6	0.688876	-4.851955	2.246429
1	3.679540	-2.557788	-3.750605
1	2.044875	-3.113015	-4.131151
6	2.598283	0.619763	-2.434020

6	4.236172	-0.722129	-1.290965
6	1.312180	0.437052	-3.116036
6	-0.183793	-1.371158	-3.665548
6	4.375357	-4.436793	-2.084740
6	2.291931	-5.375162	-3.086759
1	2.272359	-5.622793	-0.022492
1	-0.973801	-4.129699	3.515106
1	0.603271	-3.434926	3.904557
6	-2.198934	-1.018543	2.346199
6	-2.710489	-3.086438	1.224027
6	-1.034823	-0.352916	2.947269
6	1.312307	-0.789610	3.259064
6	-0.238677	-6.030914	1.922101
6	1.925091	-5.370061	2.989628
6	3.273665	1.771880	-2.057644
6	4.959521	0.431219	-0.937847
1	4.590683	-1.697968	-0.959798
6	0.370207	1.357103	-3.549531
6	-1.160968	-0.452653	-4.089744
1	-0.403834	-2.441692	-3.675198
1	4.458830	-5.283411	-1.386481
1	4.924106	-4.696623	-3.002869
1	4.872506	-3.571515	-1.626319
1	2.385643	-6.267761	-2.449594

1	2.803843	-5.582660	-4.039241
1	1.223673	-5.214035	-3.294102
6	-3.499779	-0.584184	2.148581
6	-4.051467	-2.683691	1.058904
1	-2.391403	-4.056338	0.836444
6	-0.881820	0.904877	3.512298
6	1.490997	0.490949	3.815450
1	2.170106	-1.456252	3.138363
1	0.264715	-6.754731	1.263411
1	-0.534817	-6.553138	2.844852
1	-1.151650	-5.690522	1.413384
1	2.453302	-6.133099	2.397811
1	1.634864	-5.827280	3.948149
1	2.628739	-4.549865	3.195664
6	4.453504	1.701099	-1.302745
1	2.854532	2.744802	-2.321572
6	6.316492	0.265516	-0.247529
6	-0.878741	0.930594	-4.029761
1	0.584372	2.424492	-3.468464
6	-2.500245	-1.012376	-4.580043
6	-4.439483	-1.398090	1.490761
1	-3.794268	0.406345	2.504112
6	-5.023917	-3.682232	0.419650
6	0.374920	1.344602	3.962188

1	-1.745685	1.568898	3.591748
6	2.900529	0.898510	4.251607
6	5.076880	3.014619	-0.814845
6	6.674000	1.546914	0.518588
6	6.326643	-0.901849	0.747486
6	7.368208	-0.022191	-1.335278
6	-1.919008	1.998622	-4.377830
6	-2.304491	-1.622809	-5.977981
6	-3.568088	0.091328	-4.632003
6	-3.012260	-2.100426	-3.624840
6	-5.851918	-0.842088	1.283529
6	-6.472762	-3.197043	0.581324
6	-4.695994	-3.848837	-1.072077
6	-4.906941	-5.052648	1.105594
6	0.467576	2.754403	4.562141
6	2.977941	2.423000	4.408094
6	3.239720	0.198010	5.578679
6	3.942021	0.480591	3.205038
6	6.519060	2.795917	-0.332162
6	5.108758	4.074329	-1.924919
6	4.214007	3.541182	0.347338
1	7.707923	1.462920	0.890686
1	6.025439	1.615558	1.407764
1	5.496057	-0.819222	1.461375

1	7.270957	-0.892541	1.312972
1	6.257438	-1.878756	0.248450
1	7.121311	-0.956323	-1.861566
1	8.367279	-0.132082	-0.884134
1	7.408830	0.776981	-2.088154
6	-3.043297	1.385989	-5.224522
6	-2.483389	2.564098	-3.061800
6	-1.300245	3.149877	-5.182854
1	-1.527889	-2.401541	-5.954771
1	-3.242114	-2.081065	-6.330028
1	-1.990831	-0.864318	-6.709454
1	-3.938354	0.278389	-3.610817
1	-4.429574	-0.280528	-5.209840
1	-3.004916	-1.737806	-2.585283
1	-4.045190	-2.371801	-3.894511
1	-2.412041	-3.020297	-3.668824
6	-6.620907	-1.715814	0.281948
6	-5.793645	0.585334	0.715074
6	-6.588606	-0.802550	2.632977
1	-6.807526	-3.399884	1.611889
1	-7.121770	-3.795309	-0.077975
1	-3.643434	-4.134638	-1.216859
1	-5.329965	-4.632703	-1.515426
1	-4.861989	-2.915048	-1.625214

1	-5.030863	-4.957981	2.194515
1	-5.692003	-5.724368	0.724966
1	-3.937782	-5.533736	0.911303
6	1.830763	2.971043	5.237135
6	-0.621041	2.963274	5.625686
6	0.271771	3.795114	3.446723
1	3.947826	2.687254	4.859535
1	2.961296	2.879686	3.403616
1	3.198369	-0.894433	5.455218
1	4.255505	0.469138	5.907487
1	2.531262	0.465282	6.374833
1	3.664484	0.838124	2.199800
1	4.923242	0.908420	3.466812
1	4.065536	-0.610248	3.157331
1	6.838473	3.686933	0.232043
1	7.185792	2.731798	-1.207397
1	5.602722	3.684711	-2.827323
1	5.670788	4.954429	-1.576313
1	4.103392	4.418539	-2.204455
1	3.164970	3.656094	0.033101
1	4.587554	4.517938	0.693438
1	4.220768	2.845167	1.199029
1	-3.855949	2.123729	-5.322296
1	-2.663138	1.203125	-6.243856

1	-1.686254	3.033100	-2.464088
1	-3.251781	3.325540	-3.271394
1	-2.928555	1.777426	-2.435520
1	-0.774245	2.772332	-6.072282
1	-2.096540	3.832758	-5.517030
1	-0.592083	3.742340	-4.587332
1	-7.682031	-1.419558	0.292838
1	-6.248366	-1.503672	-0.734289
1	-5.144881	0.629971	-0.173338
1	-6.804825	0.909834	0.424094
1	-5.418747	1.307764	1.454625
1	-6.039302	-0.180954	3.355250
1	-7.595733	-0.374913	2.507275
1	-6.688106	-1.805335	3.071389
1	1.964095	4.048763	5.422231
1	1.827228	2.486559	6.227173
1	-0.580150	2.173642	6.390627
1	-0.468879	3.934102	6.122444
1	-1.630581	2.969859	5.191658
1	-0.697801	3.660220	2.943645
1	0.302108	4.811990	3.869115
1	1.050368	3.712024	2.673718
1	2.008221	0.393742	0.534530
6	-0.427564	2.921846	0.206276

6	-0.281321	4.250809	-0.222337
6	-1.726677	2.472821	0.530892
6	-1.382506	5.099118	-0.321171
1	0.716313	4.620593	-0.468616
6	-2.813317	3.326957	0.424411
1	-1.872495	1.445828	0.870817
6	-2.672394	4.660411	0.003472
1	-1.218588	6.123446	-0.654287
1	-3.802165	2.940190	0.679140
6	-3.905689	5.564624	-0.058172
6	-3.557917	6.975470	-0.539944
1	-4.469817	7.589179	-0.576088
1	-2.846325	7.469838	0.137738
1	-3.121879	6.960174	-1.549814
6	-4.938083	4.960364	-1.023878
1	-5.232872	3.944851	-0.721250
1	-5.845015	5.583884	-1.048492
1	-4.529443	4.904731	-2.043269
6	-4.520771	5.665961	1.348108
1	-3.793208	6.079358	2.062263
1	-5.403570	6.323454	1.330980
1	-4.839750	4.681502	1.719929

Table S19**[As-Int]³**

E : -5494.87227526 Hartree

G : -5493.330873 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
33	-0.338295	-0.368202	-0.401475
6	0.951679	0.893906	0.317838
6	0.617597	2.167421	0.429405
6	0.733632	-2.013567	-0.244821
6	1.595723	-2.463483	-1.261062
6	0.529255	-2.875326	0.847259
6	2.112158	-1.684581	-2.478453
6	2.155539	-3.746100	-1.227713
6	-0.278367	-2.592013	2.117058
6	1.109926	-4.147273	0.891899
6	2.789132	-2.787775	-3.340517
6	3.043656	-0.555827	-2.034206
6	1.024799	-0.895479	-3.190967
6	2.968472	-4.065573	-2.470855
6	1.910888	-4.601047	-0.154743
6	0.001000	-3.853338	2.999672

6	-1.762477	-2.314380	1.880940
6	0.142605	-1.305847	2.822791
6	0.718058	-4.924855	2.134503
1	3.743859	-2.431809	-3.753172
1	2.134933	-3.013719	-4.195413
6	2.532870	0.693936	-2.407649
6	4.224663	-0.622478	-1.314157
6	1.258767	0.484660	-3.106011
6	-0.152095	-1.362411	-3.745434
6	4.438046	-4.344773	-2.131326
6	2.384761	-5.290687	-3.187498
1	2.336893	-5.608822	-0.135233
1	-0.929983	-4.238286	3.439360
1	0.652439	-3.559016	3.834677
6	-2.140263	-1.081927	2.443669
6	-2.704360	-3.075436	1.216598
6	-0.949694	-0.453188	3.032605
6	1.404495	-0.918209	3.230490
6	-0.227459	-6.075641	1.762838
6	1.945287	-5.488747	2.857856
6	3.176703	1.858049	-2.011612
6	4.920557	0.543927	-0.951060
1	4.617417	-1.594672	-1.017372
6	0.282719	1.380533	-3.516693

6	-1.158738	-0.470635	-4.156947
1	-0.324212	-2.440015	-3.801652
1	4.523568	-5.211796	-1.458862
1	5.008189	-4.565593	-3.046631
1	4.910998	-3.486862	-1.634870
1	2.478990	-6.195405	-2.567786
1	2.916273	-5.470985	-4.134795
1	1.318233	-5.139297	-3.410655
6	-3.438913	-0.621278	2.302207
6	-4.040036	-2.640124	1.093666
1	-2.406758	-4.024273	0.764803
6	-0.763807	0.776687	3.647775
6	1.614928	0.331517	3.842853
1	2.250031	-1.586696	3.049227
1	0.264553	-6.779246	1.074320
1	-0.532384	-6.630278	2.663600
1	-1.134445	-5.698918	1.268820
1	2.461842	-6.237819	2.238578
1	1.647672	-5.976736	3.798752
1	2.661525	-4.687871	3.094287
6	4.367157	1.806301	-1.273129
1	2.725201	2.823045	-2.249352
6	6.304947	0.408927	-0.310386
6	-0.943642	0.919990	-4.022971

1	0.448564	2.451728	-3.387787
6	-2.451422	-1.064825	-4.725755
6	-4.401893	-1.379464	1.612566
1	-3.711716	0.350077	2.721642
6	-5.033463	-3.568982	0.385944
6	0.513418	1.187882	4.065132
1	-1.618411	1.441310	3.793158
6	3.039621	0.695294	4.269421
6	4.950479	3.124318	-0.748453
6	6.631283	1.672003	0.498815
6	6.403750	-0.800043	0.627854
6	7.329443	0.217619	-1.444961
6	-2.044288	1.948690	-4.295307
6	-2.185895	-1.538270	-6.165027
6	-3.581437	-0.023917	-4.713419
6	-2.915568	-2.262014	-3.883275
6	-5.808669	-0.790185	1.466038
6	-6.473215	-3.079315	0.603827
6	-4.718537	-3.609030	-1.117523
6	-4.931344	-4.995052	0.949068
6	0.648629	2.578770	4.698610
6	3.151021	2.208343	4.499456
6	3.385929	-0.073784	5.556471
6	4.056754	0.308936	3.188062

6	6.408986	2.946022	-0.298746
6	4.919227	4.226708	-1.815868
6	4.089432	3.570278	0.448502
1	7.676438	1.614584	0.843681
1	6.002008	1.680489	1.404290
1	5.596725	-0.790931	1.372330
1	7.366393	-0.771677	1.160794
1	6.362289	-1.754986	0.085065
1	7.108976	-0.706413	-1.999913
1	8.348516	0.140349	-1.033344
1	7.303703	1.046291	-2.165811
6	-3.127118	1.341282	-5.197667
6	-2.645858	2.363820	-2.939268
6	-1.497066	3.201919	-4.991812
1	-1.364850	-2.270148	-6.184564
1	-3.085782	-2.017314	-6.582031
1	-1.899878	-0.702798	-6.819769
1	-3.975812	0.062227	-3.687656
1	-4.411530	-0.399512	-5.333293
1	-2.924135	-2.000058	-2.814905
1	-3.935667	-2.553514	-4.179339
1	-2.273690	-3.144710	-4.013944
6	-6.606138	-1.578444	0.417122
6	-5.736928	0.673263	0.999796

6	-6.524641	-0.837261	2.826389
1	-6.796284	-3.354472	1.621325
1	-7.138962	-3.618777	-0.088666
1	-3.678844	-3.922643	-1.293960
1	-5.384022	-4.322808	-1.628274
1	-4.847472	-2.621856	-1.582264
1	-5.047087	-4.993708	2.042988
1	-5.728475	-5.620314	0.517828
1	-3.970797	-5.471184	0.706275
6	2.023483	2.741821	5.364071
6	-0.421927	2.797408	5.778090
6	0.469489	3.645064	3.604116
1	4.129816	2.428372	4.955387
1	3.138697	2.715105	3.519723
1	3.318788	-1.158186	5.383475
1	4.412683	0.160827	5.879146
1	2.696861	0.171228	6.376542
1	3.773414	0.720534	2.205400
1	5.050055	0.704322	3.455083
1	4.158327	-0.780330	3.084157
1	6.701677	3.826585	0.295551
1	7.062370	2.944622	-1.186179
1	5.409866	3.892713	-2.742128
1	5.453221	5.114205	-1.442861

1	3.895779	4.541656	-2.062615
1	3.032153	3.664965	0.156054
1	4.437758	4.541813	0.833530
1	4.131746	2.836426	1.267120
1	-3.980634	2.036736	-5.243910
1	-2.733215	1.262175	-6.224990
1	-1.879052	2.827680	-2.299975
1	-3.457315	3.094110	-3.089064
1	-3.045059	1.501503	-2.385432
1	-0.936129	2.937835	-5.900645
1	-2.334857	3.854989	-5.280949
1	-0.839569	3.789296	-4.335833
1	-7.662848	-1.270937	0.469204
1	-6.248797	-1.296601	-0.587347
1	-5.096224	0.773019	0.109935
1	-6.746741	1.030370	0.744120
1	-5.344807	1.336242	1.784741
1	-5.953483	-0.279896	3.583334
1	-7.525528	-0.384373	2.748306
1	-6.636035	-1.867741	3.191689
1	2.179685	3.808400	5.591258
1	2.021028	2.216768	6.333347
1	-0.399710	1.989088	6.524060
1	-0.232435	3.750528	6.295660

1	-1.435267	2.849296	5.356347
1	-0.511615	3.545611	3.115658
1	0.535772	4.653539	4.042305
1	1.231179	3.551817	2.815457
1	1.943765	0.513164	0.593228
6	-0.527794	3.018826	0.268172
6	-0.429190	4.283981	-0.332449
6	-1.796915	2.602054	0.726075
6	-1.551095	5.098134	-0.477547
1	0.545438	4.628633	-0.684659
6	-2.904712	3.421911	0.572755
1	-1.898916	1.622532	1.199072
6	-2.812922	4.689234	-0.027787
1	-1.426130	6.071450	-0.951138
1	-3.870495	3.062083	0.933074
6	-4.064211	5.564600	-0.134754
6	-3.781044	6.880747	-0.863611
1	-4.706633	7.470401	-0.935088
1	-3.036901	7.488324	-0.327960
1	-3.413577	6.703222	-1.885364
6	-5.161521	4.810277	-0.903055
1	-5.420153	3.858317	-0.417010
1	-6.075208	5.421998	-0.955296
1	-4.835771	4.589047	-1.929681

6	-4.566307	5.887043	1.283075
1	-3.793154	6.417152	1.858608
1	-5.462454	6.524714	1.234392
1	-4.830546	4.971881	1.832531

Table S20

[Sb-Int]³

E : -3499.42411789 Hartree

G : -3497.886076 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
51	-0.692827	-0.306736	-0.150172
6	0.773153	1.149395	0.648760
6	0.542793	2.418080	0.519479
6	0.629920	-2.068720	-0.171294
6	1.419705	-2.412782	-1.283685
6	0.593017	-3.003471	0.879634
6	1.821220	-1.532426	-2.471305
6	2.066776	-3.653231	-1.376713
6	-0.151415	-2.883981	2.210618
6	1.266396	-4.229894	0.803436

6	2.443426	-2.547842	-3.472265
6	2.782133	-0.441434	-2.000740
6	0.711658	-0.695207	-3.082377
6	2.781086	-3.854256	-2.702936
6	1.990769	-4.574037	-0.335232
6	0.369053	-4.116849	3.018971
6	-1.668958	-2.842338	2.054988
6	0.093133	-1.590335	2.976502
6	1.074379	-5.089561	2.039474
1	3.321381	-2.119196	-3.976297
1	1.697976	-2.764824	-4.251554
6	2.306626	0.831085	-2.342193
6	3.957735	-0.562800	-1.280661
6	0.997076	0.675515	-2.991166
6	-0.498379	-1.116862	-3.602613
6	4.291328	-4.056671	-2.523656
6	2.204033	-5.074958	-3.432889
1	2.490068	-5.545121	-0.408548
1	-0.446656	-4.601225	3.574435
1	1.097184	-3.759197	3.761036
6	-2.218132	-1.754247	2.754744
6	-2.495841	-3.668631	1.318826
6	-1.113404	-0.966745	3.324500
6	1.298484	-1.012460	3.332169

6	0.204038	-6.313780	1.723777
6	2.418628	-5.560229	2.605589
6	3.017360	1.961385	-1.963336
6	4.703185	0.569456	-0.909481
1	4.299165	-1.553513	-0.980490
6	0.038470	1.607398	-3.364417
6	-1.489931	-0.188603	-3.967499
1	-0.704496	-2.188194	-3.671372
1	4.495139	-4.930376	-1.886114
1	4.770469	-4.228786	-3.499630
1	4.769235	-3.180883	-2.065213
1	2.417920	-6.003499	-2.881843
1	2.645738	-5.166585	-4.437351
1	1.112865	-4.984707	-3.539309
6	-3.584048	-1.523226	2.715411
6	-3.888469	-3.461560	1.283167
1	-2.058002	-4.478395	0.731690
6	-1.094243	0.243441	4.003617
6	1.335567	0.217522	4.013443
1	2.228970	-1.507843	3.044434
1	0.669780	-6.933222	0.942352
1	0.075423	-6.934571	2.623803
1	-0.793414	-6.015710	1.373002
1	2.925130	-6.244840	1.908244

1	2.269716	-6.096467	3.555557
1	3.085533	-4.704988	2.790263
6	4.213186	1.854909	-1.238112
1	2.623332	2.946614	-2.215220
6	6.068443	0.360247	-0.247457
6	-1.219382	1.192422	-3.833260
1	0.245353	2.671705	-3.240750
6	-2.819956	-0.737980	-4.497547
6	-4.437746	-2.361915	1.976418
1	-3.997637	-0.664059	3.247095
6	-4.733853	-4.435542	0.455573
6	0.121157	0.855317	4.355424
1	-2.037755	0.737088	4.246701
6	2.691662	0.821034	4.386404
6	4.872602	3.144383	-0.734105
6	6.477759	1.622235	0.524310
6	6.063674	-0.818816	0.733900
6	7.091174	0.055435	-1.358005
6	-2.296375	2.253580	-4.068949
6	-2.593345	-1.275798	-5.921042
6	-3.904634	0.351405	-4.520887
6	-3.331696	-1.879947	-3.606039
6	-5.936158	-2.038915	1.970273
6	-6.220803	-4.278112	0.805171

6	-4.507605	-4.154571	-1.039454
6	-4.335049	-5.890375	0.747566
6	0.050949	2.229691	5.037970
6	2.541234	2.342042	4.523653
6	3.163279	0.188498	5.708590
6	3.761946	0.543669	3.324048
6	6.325042	2.885841	-0.305540
6	4.886669	4.235462	-1.813516
6	4.058103	3.653710	0.469876
1	7.520171	1.509905	0.863838
1	5.858280	1.694035	1.433971
1	5.246286	-0.721950	1.460994
1	7.016497	-0.841327	1.284631
1	5.959440	-1.787627	0.225247
1	6.806561	-0.863151	-1.892748
1	8.094096	-0.091698	-0.926480
1	7.143469	0.863778	-2.100310
6	-3.383201	1.695261	-4.996968
6	-2.887271	2.625026	-2.696204
6	-1.726945	3.525681	-4.710535
1	-1.802179	-2.039958	-5.927012
1	-3.517592	-1.732463	-6.308371
1	-2.285639	-0.474497	-6.608250
1	-4.325364	0.462349	-3.508738

1	-4.732665	0.006418	-5.160821
1	-3.357051	-1.566730	-2.550801
1	-4.353176	-2.158808	-3.909597
1	-2.711039	-2.784225	-3.678576
6	-6.650142	-2.823012	0.858730
6	-6.174252	-0.543572	1.709376
6	-6.531174	-2.402552	3.341320
1	-6.410845	-4.756471	1.780369
1	-6.819846	-4.832972	0.065354
1	-3.439641	-4.233304	-1.292643
1	-5.062316	-4.881020	-1.654184
1	-4.835997	-3.143108	-1.315403
1	-4.366889	-6.097282	1.827552
1	-5.037205	-6.572897	0.244280
1	-3.326559	-6.129009	0.381300
6	1.437673	2.712146	5.497932
6	-0.863612	2.177439	6.270660
6	-0.523016	3.242040	4.031924
1	3.502369	2.771868	4.849257
1	2.324054	2.762122	3.525231
1	3.323042	-0.891479	5.572412
1	4.113687	0.640035	6.035561
1	2.422862	0.309475	6.510863
1	3.436833	0.860621	2.319901

1	4.679611	1.099019	3.575220
1	4.031450	-0.520327	3.279420
1	6.685173	3.761333	0.258367
1	6.959144	2.817034	-1.204516
1	5.341075	3.865105	-2.744378
1	5.475541	5.095388	-1.459228
1	3.878388	4.606606	-2.046067
1	3.007451	3.823481	0.189452
1	4.477476	4.601275	0.843581
1	4.055441	2.924933	1.293777
1	-4.206565	2.424917	-5.060236
1	-2.968199	1.600942	-6.015008
1	-2.114306	3.092311	-2.067250
1	-3.718495	3.339628	-2.810804
1	-3.256353	1.741347	-2.155734
1	-1.166331	3.293865	-5.628466
1	-2.554470	4.202883	-4.974378
1	-1.065526	4.073469	-4.023772
1	-7.738115	-2.744201	1.013865
1	-6.440248	-2.339878	-0.109837
1	-5.653852	-0.217899	0.796281
1	-7.251879	-0.360000	1.578031
1	-5.833364	0.086870	2.542260
1	-6.020786	-1.849346	4.143374

1	-7.601957	-2.147123	3.374028
1	-6.421604	-3.474342	3.559201
1	1.396997	3.803309	5.641885
1	1.666961	2.284506	6.486650
1	-0.528490	1.400514	6.973989
1	-0.838926	3.147576	6.791079
1	-1.909592	1.969725	6.004629
1	-1.527303	2.937586	3.703079
1	-0.605180	4.237154	4.496053
1	0.111084	3.322084	3.136000
1	1.621436	0.693938	1.172005
6	-0.249775	3.506008	0.079684
6	0.201661	4.389744	-0.924895
6	-1.526433	3.756546	0.640091
6	-0.582968	5.454789	-1.351911
1	1.188827	4.233147	-1.360700
6	-2.295735	4.822969	0.200808
1	-1.902058	3.084933	1.413285
6	-1.849713	5.700989	-0.803549
1	-0.185342	6.106491	-2.129558
1	-3.280372	4.972047	0.649570
6	-2.738285	6.863456	-1.252261
6	-2.056004	7.726404	-2.317469
1	-2.724558	8.549511	-2.609049

1	-1.120830	8.167861	-1.942403
1	-1.826954	7.143833	-3.222331
6	-4.041866	6.305607	-1.846665
1	-4.579154	5.673188	-1.125015
1	-4.709786	7.129622	-2.141680
1	-3.828428	5.697203	-2.737998
6	-3.064710	7.752436	-0.040899
1	-2.143440	8.154211	0.406033
1	-3.698286	8.598001	-0.349898
1	-3.603831	7.194417	0.737780

Table S21

[Bi-Int]³

E : -3473.78080259 Hartree

G : -3472.242875 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
83	-1.177453	-0.507566	-0.672876
6	1.543000	1.380685	0.771912
6	0.597686	2.135245	0.693666
6	0.463738	-2.102487	-0.305701

6	1.397185	-2.472782	-1.290372
6	0.443960	-2.896300	0.857375
6	1.897424	-1.667081	-2.500734
6	2.145333	-3.656854	-1.195179
6	-0.335403	-2.648254	2.155180
6	1.246354	-4.038451	0.988311
6	2.621981	-2.735779	-3.364055
6	2.826022	-0.559054	-1.998314
6	0.862203	-0.852212	-3.252967
6	2.915331	-3.972935	-2.467773
6	2.074504	-4.451099	-0.054325
6	-0.112826	-3.969579	2.957814
6	-1.817282	-2.346154	1.996220
6	0.132744	-1.394645	2.898521
6	1.071635	-4.742175	2.321887
1	3.534487	-2.322198	-3.816982
1	1.956344	-3.027445	-4.189961
6	2.360854	0.705547	-2.380653
6	3.994817	-0.663610	-1.263419
6	1.108932	0.524694	-3.128583
6	-0.260574	-1.291044	-3.930736
6	4.413556	-4.198493	-2.231683
6	2.328836	-5.241749	-3.106197
1	2.650578	-5.378446	0.021375

1	-1.025584	-4.577541	2.875928
1	0.044466	-3.765145	4.026643
6	-2.170322	-1.151361	2.642267
6	-2.769322	-3.054715	1.288851
6	-0.953114	-0.565489	3.220737
6	1.410210	-1.005656	3.261023
6	0.714886	-6.220510	2.127028
6	2.348417	-4.645835	3.168488
6	3.063051	1.847151	-2.013454
6	4.755826	0.474987	-0.943893
1	4.333730	-1.646518	-0.937730
6	0.180175	1.439662	-3.599826
6	-1.216448	-0.378090	-4.413571
1	-0.435212	-2.364710	-4.031442
1	4.576673	-5.020615	-1.518380
1	4.910242	-4.468675	-3.176147
1	4.910860	-3.302352	-1.838231
1	2.494333	-6.119134	-2.462507
1	2.802417	-5.436835	-4.081208
1	1.245120	-5.131853	-3.259608
6	-3.463896	-0.663609	2.535874
6	-4.081136	-2.564270	1.150835
1	-2.475069	-3.974655	0.776306
6	-0.747862	0.620286	3.912294

6	1.636046	0.186569	3.975331
1	2.257249	-1.626854	2.966901
1	1.548904	-6.773641	1.668832
1	0.489640	-6.692738	3.095891
1	-0.165116	-6.326880	1.475528
1	3.198045	-5.108401	2.643635
1	2.212274	-5.166575	4.128960
1	2.610611	-3.601403	3.384081
6	4.268329	1.754968	-1.300418
1	2.662287	2.828034	-2.276215
6	6.149244	0.280744	-0.339361
6	-1.006633	1.005593	-4.214369
1	0.349670	2.505966	-3.439301
6	-2.449633	-0.931598	-5.134386
6	-4.425405	-1.338603	1.762263
1	-3.725180	0.277472	3.025328
6	-5.043569	-3.344449	0.250946
6	0.540175	1.011747	4.310257
1	-1.601172	1.263363	4.140405
6	3.064848	0.518474	4.416332
6	4.953645	3.054944	-0.856074
6	6.564827	1.546074	0.422616
6	6.216083	-0.909998	0.623827
6	7.124426	0.005186	-1.500381

6	-2.074312	2.058065	-4.530390
6	-2.058717	-1.268242	-6.584026
6	-3.585628	0.101693	-5.114253
6	-2.969667	-2.207375	-4.455819
6	-5.813910	-0.703275	1.626063
6	-6.484244	-2.854367	0.453165
6	-4.609863	-3.135184	-1.210707
6	-5.008630	-4.846300	0.568195
6	0.688849	2.363285	5.021612
6	3.185840	2.019785	4.709095
6	3.389274	-0.311048	5.672127
6	4.094985	0.169165	3.337463
6	6.405990	2.800757	-0.419658
6	4.980314	4.093083	-1.986683
6	4.158521	3.635345	0.327534
1	7.610745	1.438385	0.752843
1	5.953407	1.623197	1.337809
1	5.437408	-0.842857	1.393985
1	7.196413	-0.920879	1.124116
1	6.105829	-1.873270	0.106083
1	6.844082	-0.927089	-2.013163
1	8.152966	-0.103805	-1.120681
1	7.109494	0.807524	-2.250517
6	-3.119716	1.493892	-5.503027

6	-2.749245	2.461175	-3.204469
6	-1.464655	3.314952	-5.167006
1	-1.242423	-2.005517	-6.597564
1	-2.919077	-1.694756	-7.123752
1	-1.709070	-0.379893	-7.128506
1	-4.023617	0.123972	-4.101970
1	-4.385981	-0.239895	-5.790282
1	-3.080886	-2.055073	-3.371654
1	-3.953622	-2.472935	-4.872598
1	-2.305614	-3.068481	-4.614679
6	-6.583645	-1.339733	0.458964
6	-5.700624	0.802140	1.336170
6	-6.586490	-0.896763	2.941728
1	-6.867034	-3.254694	1.406635
1	-7.119011	-3.281267	-0.339776
1	-3.575891	-3.482918	-1.361155
1	-5.266788	-3.694863	-1.895795
1	-4.636292	-2.071335	-1.490832
1	-5.203744	-5.026011	1.635774
1	-5.784505	-5.364406	-0.016344
1	-4.043758	-5.305452	0.312655
6	2.089387	2.513330	5.635244
6	-0.336231	2.507022	6.156089
6	0.452609	3.484698	3.994367

1	4.178892	2.220434	5.142782
1	3.141253	2.567019	3.751626
1	3.338473	-1.385451	5.439551
1	4.404687	-0.082999	6.033599
1	2.675719	-0.118579	6.484983
1	3.856242	0.661023	2.381445
1	5.093453	0.511953	3.652475
1	4.164876	-0.913401	3.162840
1	6.761944	3.683611	0.135233
1	7.044931	2.724761	-1.314048
1	5.431127	3.671731	-2.897468
1	5.580333	4.961631	-1.674231
1	3.976772	4.462969	-2.238903
1	3.107081	3.800927	0.051349
1	4.595782	4.594715	0.646243
1	4.157658	2.949829	1.188733
1	-3.974348	2.188388	-5.544645
1	-2.689416	1.471727	-6.517962
1	-2.005987	2.830082	-2.480478
1	-3.484933	3.262538	-3.383505
1	-3.267288	1.611330	-2.734405
1	-0.849065	3.056788	-6.041357
1	-2.271921	3.985771	-5.499253
1	-0.841919	3.880530	-4.459780

1	-7.636553	-1.019687	0.514172
1	-6.187396	-0.939368	-0.488946
1	-5.021189	0.987351	0.488777
1	-6.693246	1.204980	1.080481
1	-5.333051	1.366607	2.205660
1	-6.035133	-0.451018	3.782730
1	-7.574025	-0.412920	2.881291
1	-6.733314	-1.961406	3.171741
1	2.247470	3.572709	5.893034
1	2.132041	1.956546	6.585427
1	-0.272324	1.658844	6.853930
1	-0.135479	3.432304	6.718134
1	-1.367829	2.567991	5.782360
1	-0.545078	3.395598	3.538707
1	0.520101	4.469025	4.484084
1	1.186016	3.444581	3.175712
1	2.367144	0.686679	0.781564
6	-0.556205	2.971290	0.514222
6	-0.494658	4.126058	-0.274680
6	-1.792980	2.611317	1.078301
6	-1.636736	4.893525	-0.503804
1	0.458708	4.416126	-0.719697
6	-2.920930	3.385213	0.844339
1	-1.855481	1.709720	1.690921

6	-2.874885	4.537476	0.042766
1	-1.547145	5.778844	-1.132609
1	-3.865520	3.075731	1.294610
6	-4.152106	5.350962	-0.180621
6	-3.943725	6.468654	-1.206042
1	-4.889765	7.006582	-1.364037
1	-3.197360	7.200495	-0.864250
1	-3.615746	6.065705	-2.176361
6	-5.271851	4.428183	-0.689955
1	-5.516608	3.640128	0.036519
1	-6.187329	5.011649	-0.871189
1	-4.978917	3.940599	-1.631279
6	-4.578954	5.977909	1.157252
1	-3.793870	6.644385	1.543664
1	-5.501037	6.565162	1.026902
1	-4.771084	5.204775	1.915521

Table S22

[N-T/S]

E : -3313.91011 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

7	0.441452	-0.486095	-0.243793
6	1.134466	0.457726	0.291475
6	0.986695	1.843042	-0.061175
6	0.901513	-1.808375	-0.190485
6	1.617866	-2.325878	-1.280673
6	0.617188	-2.695669	0.862057
6	2.056910	-1.544627	-2.502007
6	2.029984	-3.656831	-1.331492
6	-0.255022	-2.435397	2.079670
6	1.077840	-4.016078	0.832820
6	2.487754	-2.683229	-3.477176
6	3.144562	-0.525591	-2.164369
6	0.977806	-0.630444	-3.064557
6	2.723695	-3.978224	-2.646852
6	1.779877	-4.518269	-0.263257
6	0.003853	-3.695364	2.964851
6	-1.719316	-2.253746	1.687334
6	0.015100	-1.123715	2.801067
6	0.734625	-4.769083	2.108104
1	3.368796	-2.398592	-4.070148
1	1.661076	-2.854533	-4.182837
6	2.793058	0.753774	-2.619179
6	4.289475	-0.690029	-1.404276

6	1.437390	0.688557	-3.185125
6	-0.356493	-0.919310	-3.266191
6	4.215597	-4.271624	-2.437898
6	2.070381	-5.187454	-3.325669
1	2.118796	-5.557660	-0.285133
1	-0.937890	-4.075784	3.385392
1	0.638949	-3.403988	3.813868
6	-2.223880	-1.032035	2.158957
6	-2.545943	-3.116051	0.993070
6	-1.134252	-0.320321	2.846134
6	1.204964	-0.655956	3.325084
6	-0.149911	-5.990013	1.827218
6	2.018975	-5.232090	2.809406
6	3.597384	1.842697	-2.316413
6	5.116215	0.402310	-1.088104
1	4.522125	-1.675099	-0.998760
6	0.572639	1.682262	-3.623154
6	-1.269777	0.099849	-3.586226
1	-0.718008	-1.931312	-3.062159
1	4.351022	-5.120954	-1.751080
1	4.692345	-4.526413	-3.396791
1	4.743642	-3.405175	-2.018751
1	2.224941	-6.104217	-2.736503
1	2.506639	-5.350230	-4.323450

1	0.987350	-5.032801	-3.439324
6	-3.542181	-0.682032	1.896765
6	-3.902522	-2.809496	0.775452
1	-2.139442	-4.056211	0.614077
6	-1.072112	0.941485	3.418385
6	1.299076	0.640785	3.865795
1	2.095802	-1.286783	3.263857
1	0.360727	-6.696821	1.155813
1	-0.383921	-6.517944	2.764351
1	-1.099012	-5.700566	1.355534
1	2.565246	-5.962693	2.193751
1	1.782113	-5.707160	3.774215
1	2.686670	-4.378326	2.997522
6	4.760628	1.690170	-1.548172
1	3.274793	2.840913	-2.617728
6	6.397602	0.138906	-0.291410
6	-0.784252	1.396901	-3.855999
1	0.939521	2.704444	-3.745277
6	-2.763021	-0.228070	-3.495027
6	-4.395840	-1.555715	1.198145
1	-3.922115	0.279974	2.250676
6	-4.777547	-3.886363	0.119358
6	0.136362	1.440962	3.934325
1	-1.966971	1.567585	3.437964

6	2.666849	1.123413	4.362016
6	5.513676	2.958475	-1.128134
6	6.871836	1.432292	0.386520
6	6.185596	-0.913892	0.805148
6	7.471265	-0.382632	-1.263310
6	-1.686096	2.522102	-4.374360
6	-3.167680	-1.227395	-4.588605
6	-3.599379	1.055757	-3.610650
6	-3.055047	-0.845194	-2.117301
6	-5.841354	-1.113793	0.946033
6	-6.262618	-3.500683	0.203951
6	-4.375156	-4.089358	-1.350746
6	-4.598451	-5.223025	0.858301
6	0.132215	2.865229	4.501571
6	2.661211	2.650120	4.528312
6	2.986022	0.437967	5.701743
6	3.775784	0.771755	3.358174
6	6.901790	2.612978	-0.568467
6	5.709739	3.915068	-2.312334
6	4.679526	3.672264	-0.048020
1	7.871111	1.261596	0.819221
1	6.198912	1.652122	1.232737
1	5.326754	-0.651672	1.439771
1	7.082688	-0.966713	1.441184

1	6.016879	-1.920003	0.396398
1	7.133604	-1.318061	-1.734189
1	8.412199	-0.583851	-0.726530
1	7.673902	0.335415	-2.069985
6	-3.082737	1.973329	-4.703917
6	-1.797430	3.624439	-3.312751
6	-1.093368	3.120697	-5.658399
1	-2.552418	-2.137542	-4.534879
1	-4.222493	-1.520898	-4.465734
1	-3.042136	-0.799709	-5.593817
1	-3.571822	1.585757	-2.642103
1	-4.652412	0.781034	-3.785876
1	-2.688545	-0.194210	-1.308416
1	-4.142930	-0.973988	-1.992168
1	-2.585321	-1.829771	-1.983893
6	-6.495755	-2.031383	-0.097651
6	-5.889001	0.322523	0.401635
6	-6.626477	-1.160355	2.267783
1	-6.639146	-3.732322	1.213614
1	-6.833284	-4.137054	-0.490952
1	-3.297506	-4.293815	-1.440603
1	-4.921726	-4.946531	-1.773496
1	-4.597000	-3.203407	-1.960708
1	-4.770924	-5.100694	1.937823

1	-5.321858	-5.957913	0.472605
1	-3.592502	-5.643094	0.716760
6	1.432680	3.146562	5.268616
6	-1.038475	3.069299	5.474669
6	-0.018989	3.854461	3.334308
1	3.580770	2.952562	5.054439
1	2.706913	3.115133	3.528988
1	2.991549	-0.655653	5.582863
1	3.978292	0.749842	6.063821
1	2.240598	0.681667	6.471809
1	3.541493	1.157453	2.352855
1	4.725271	1.226381	3.682552
1	3.942952	-0.311798	3.283395
1	7.310082	3.504800	-0.065660
1	7.583836	2.392700	-1.405989
1	6.193631	3.402316	-3.156831
1	6.351766	4.755178	-2.004628
1	4.760520	4.340039	-2.666478
1	3.659739	3.867935	-0.410401
1	5.151938	4.628079	0.230362
1	4.581931	3.054014	0.856296
1	-3.769610	2.819717	-4.867490
1	-3.036514	1.419364	-5.656568
1	-0.809647	4.044681	-3.073128

1	-2.440186	4.445837	-3.671600
1	-2.216081	3.229491	-2.376773
1	-0.942279	2.340454	-6.418787
1	-1.780753	3.876853	-6.069634
1	-0.126232	3.609643	-5.475117
1	-7.573712	-1.808151	-0.142287
1	-6.085369	-1.788618	-1.092642
1	-5.232083	0.433059	-0.475507
1	-6.917338	0.572337	0.097652
1	-5.586734	1.060375	1.159748
1	-6.165959	-0.495814	3.013621
1	-7.665646	-0.831702	2.109160
1	-6.642239	-2.171958	2.696305
1	1.504083	4.229481	5.457870
1	1.378157	2.662925	6.257809
1	-1.028712	2.307324	6.268007
1	-0.953761	4.060350	5.946951
1	-2.013714	3.027555	4.969656
1	-0.939216	3.647147	2.765054
1	-0.068856	4.889083	3.709115
1	0.820876	3.777345	2.628537
1	2.011991	0.229799	0.925986
6	-0.279704	2.495534	0.059598
6	-0.326212	3.895152	-0.122601

6	-1.499308	1.815397	0.300758
6	-1.519907	4.597042	-0.024021
1	0.615556	4.407610	-0.328614
6	-2.694040	2.511352	0.329982
1	-1.483597	0.732144	0.421552
6	-2.729011	3.913104	0.182129
1	-1.510539	5.678514	-0.147155
1	-3.621173	1.954803	0.474286
6	-4.080210	4.622575	0.226859
6	-3.950685	6.128960	-0.011952
1	-4.948249	6.590769	0.008505
1	-3.339836	6.612052	0.764494
1	-3.501103	6.343383	-0.992608
6	-4.987272	4.027142	-0.865130
1	-5.169530	2.954600	-0.705719
1	-5.960633	4.540149	-0.863633
1	-4.533647	4.150250	-1.860219
6	-4.711040	4.390051	1.610485
1	-4.067409	4.795158	2.405780
1	-5.690303	4.889007	1.667622
1	-4.862611	3.319100	1.808738

Table S23

[P-T/S]

E : -3600.448747 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
15	-0.026622	0.130940	0.219375
6	-0.128805	0.168205	2.032357
6	1.065654	-0.169583	2.424458
6	-1.728721	-0.600098	-0.021386
6	-2.031451	-1.970261	-0.006684
6	-2.813956	0.285391	-0.201959
6	-1.063918	-3.134330	0.132363
6	-3.347258	-2.435731	-0.144848
6	-2.764194	1.792202	-0.465038
6	-4.130412	-0.179133	-0.294283
6	-1.937505	-4.347237	-0.326430
6	-0.465856	-3.312556	1.527222
6	0.199504	-3.037891	-0.703429
6	-3.426602	-3.953383	-0.166485
6	-4.409491	-1.544941	-0.264540
6	-4.259610	2.217338	-0.357364
6	-2.134602	2.060706	-1.833890
6	-1.858105	2.620835	0.438567

6	-5.146439	0.943194	-0.422102
1	-1.676398	-5.264918	0.219553
1	-1.728039	-4.524637	-1.391838
6	0.910633	-3.590332	1.439334
6	-1.050720	-3.167838	2.769816
6	1.327226	-3.413428	0.039356
6	0.339752	-2.571676	-1.994257
6	-4.033441	-4.502780	1.132378
6	-4.256674	-4.450678	-1.354475
1	-5.437427	-1.908920	-0.354185
1	-4.518439	2.947599	-1.137595
1	-4.406603	2.717954	0.610604
6	-1.047358	2.940521	-1.724255
6	-2.489875	1.567222	-3.075832
6	-0.866543	3.277946	-0.306803
6	-1.897236	2.775018	1.812608
6	-5.940256	0.852934	-1.731743
6	-6.127473	0.903400	0.757814
6	1.650563	-3.807805	2.591581
6	-0.301332	-3.332746	3.951975
1	-2.097762	-2.864478	2.836142
6	2.581008	-3.386701	-0.557068
6	1.615247	-2.418293	-2.566139
1	-0.546972	-2.230169	-2.535731

1	-5.042927	-4.094612	1.292911
1	-4.111121	-5.599592	1.081273
1	-3.416679	-4.249865	2.004129
1	-5.316134	-4.173624	-1.243203
1	-4.203155	-5.547946	-1.425999
1	-3.886541	-4.023018	-2.297809
6	-0.336055	3.311985	-2.855922
6	-1.817595	1.978214	-4.243375
1	-3.306874	0.846573	-3.152747
6	0.103215	4.028022	0.335886
6	-0.905888	3.514558	2.487555
1	-2.687655	2.280710	2.384522
1	-6.478511	-0.104516	-1.800819
1	-6.682080	1.664522	-1.783343
1	-5.284846	0.940568	-2.608564
1	-6.739222	-0.011483	0.734201
1	-6.807971	1.768185	0.721459
1	-5.586927	0.925624	1.715739
6	1.056196	-3.702444	3.861706
1	2.719092	-4.019015	2.513707
6	-1.018123	-3.084354	5.283836
6	2.744649	-2.880969	-1.858356
1	3.457884	-3.697471	0.016180
6	1.695933	-1.675559	-3.902685

6	-0.708067	2.844285	-4.127489
1	0.517750	3.984616	-2.754484
6	-2.344039	1.457900	-5.587637
6	0.110124	4.146932	1.735703
1	0.885367	4.509145	-0.253052
6	-1.007664	3.646406	4.012820
6	1.933770	-3.930666	5.096381
6	-0.018912	-3.061176	6.451965
6	-1.728804	-1.721555	5.254388
6	-2.059210	-4.192363	5.513323
6	4.161003	-2.768037	-2.426936
6	1.005330	-2.505736	-4.996341
6	3.155500	-1.401671	-4.306519
6	0.987108	-0.317929	-3.763955
6	0.089684	3.332819	-5.341382
6	-1.700725	2.224105	-6.754481
6	-2.045690	-0.044521	-5.723053
6	-3.864986	1.662731	-5.677443
6	1.274277	4.904087	2.383175
6	0.321837	4.138795	4.604619
6	-2.133987	4.643917	4.335567
6	-1.328131	2.303617	4.684360
6	1.045195	-4.137161	6.331038
6	2.809841	-5.180473	4.929159

6	2.851593	-2.712897	5.293169
1	-0.577193	-3.166902	7.395838
1	0.465478	-2.072306	6.490653
1	-1.018591	-0.926561	4.978731
1	-2.135843	-1.491607	6.251593
1	-2.564974	-1.699030	4.540832
1	-2.771984	-4.241525	4.676944
1	-2.626599	-3.998870	6.437061
1	-1.580272	-5.178421	5.599704
6	4.087401	-2.544018	-3.944292
6	4.877322	-1.592868	-1.737561
6	4.966776	-4.050463	-2.177841
1	-0.038788	-2.726246	-4.730029
1	1.005071	-1.953676	-5.949463
1	1.521038	-3.464971	-5.152336
1	3.501653	-0.480410	-3.811746
1	3.190630	-1.197276	-5.388539
1	1.433445	0.276959	-2.951467
1	1.086233	0.249829	-4.703130
1	-0.087160	-0.414768	-3.550419
6	-0.211496	2.445394	-6.557727
6	1.602615	3.280519	-5.078589
6	-0.297716	4.793075	-5.634484
1	-2.203790	3.198259	-6.865593

1	-1.891900	1.670632	-7.687683
1	-2.445835	-0.603876	-4.863042
1	-2.513072	-0.442530	-6.637196
1	-0.966386	-0.241121	-5.773186
1	-4.131934	2.709509	-5.469111
1	-4.212596	1.411598	-6.691572
1	-4.413527	1.021892	-4.972609
6	0.921878	5.293950	3.825451
6	1.610177	6.194880	1.622375
6	2.508567	3.984374	2.360029
1	0.157190	4.422382	5.656521
1	1.035420	3.298078	4.618446
1	-3.091781	4.287498	3.928494
1	-2.243520	4.762058	5.425067
1	-1.935584	5.630880	3.894316
1	-0.558494	1.555766	4.440357
1	-1.341041	2.433923	5.777647
1	-2.308809	1.901687	4.391991
1	1.682422	-4.154990	7.229737
1	0.567929	-5.129721	6.264918
1	2.201476	-6.060563	4.673503
1	3.337929	-5.387476	5.872808
1	3.573642	-5.050659	4.149611
1	3.486904	-2.556274	4.408283

1	3.505555	-2.861757	6.167924
1	2.277053	-1.787657	5.437725
1	5.102698	-2.352723	-4.327226
1	3.739607	-3.476322	-4.421683
1	4.974722	-1.784502	-0.658655
1	5.887191	-1.453985	-2.155399
1	4.318646	-0.652448	-1.843611
1	4.442175	-4.930230	-2.578321
1	5.944407	-3.973889	-2.678169
1	5.158902	-4.222576	-1.109432
1	0.233753	2.906987	-7.453677
1	0.294249	1.473547	-6.425212
1	1.913310	2.284042	-4.733790
1	2.144593	3.508925	-6.009220
1	1.920376	4.016289	-4.326875
1	-0.069581	5.430123	-4.767238
1	0.268635	5.173158	-6.499303
1	-1.371053	4.898222	-5.844967
1	1.831294	5.664858	4.324842
1	0.212800	6.138217	3.804569
1	0.718197	6.827103	1.500321
1	2.362469	6.765862	2.187954
1	2.033149	5.998490	0.627767
1	2.776648	3.727650	1.324451

1	3.372501	4.482229	2.828686
1	2.321726	3.036841	2.883525
1	-1.069805	0.219137	2.599073
6	2.440167	-0.280833	2.708563
6	2.988440	0.468628	3.772507
6	3.314714	-1.105741	1.965800
6	4.336363	0.362852	4.098457
1	2.334633	1.112932	4.363241
6	4.651927	-1.197495	2.311468
1	2.920790	-1.641902	1.104305
6	5.200486	-0.478743	3.388432
1	4.709730	0.950836	4.936587
1	5.296981	-1.849024	1.716085
6	6.684058	-0.631779	3.723324
6	7.079702	0.194278	4.949987
1	8.149052	0.051468	5.163309
1	6.910838	1.268576	4.785561
1	6.513116	-0.112900	5.841751
6	6.987145	-2.110971	4.016140
1	6.765788	-2.749373	3.148786
1	8.051279	-2.240510	4.267039
1	6.384181	-2.470415	4.863602
6	7.520931	-0.159985	2.521975
1	7.316130	0.897785	2.299795

1	8.595420	-0.268521	2.736232
1	7.294221	-0.744131	1.618217

Table S24

[As-T/S]

E : -5494.842741 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
33	-0.018765	0.133556	0.159383
6	-0.097157	0.223319	2.118061
6	1.095527	-0.151630	2.437661
6	-1.836937	-0.666785	0.002469
6	-2.133185	-2.036463	0.080763
6	-2.931635	0.207971	-0.174983
6	-1.162845	-3.196543	0.243391
6	-3.451245	-2.511884	0.003647
6	-2.907261	1.706331	-0.501317
6	-4.248420	-0.266631	-0.206396
6	-2.044174	-4.428794	-0.141010
6	-0.544754	-3.318646	1.633475
6	0.085708	-3.140909	-0.615680

6	-3.529341	-4.028939	0.034758
6	-4.520430	-1.630207	-0.113032
6	-4.403451	2.121866	-0.370346
6	-2.319313	1.927728	-1.896487
6	-1.989175	2.582230	0.343068
6	-5.278141	0.839648	-0.354926
1	-1.768903	-5.320330	0.440282
1	-1.859398	-4.655625	-1.201493
6	0.828734	-3.606863	1.538874
6	-1.117587	-3.126088	2.874307
6	1.225081	-3.483776	0.125595
6	0.202318	-2.734809	-1.929441
6	-4.115496	-4.535032	1.359884
6	-4.378563	-4.562896	-1.123811
1	-5.549619	-2.000018	-0.152693
1	-4.690134	2.813331	-1.175455
1	-4.529771	2.664568	0.577605
6	-1.242088	2.826426	-1.852957
6	-2.697710	1.374490	-3.106559
6	-1.026231	3.220076	-0.454116
6	-1.992061	2.784897	1.712561
6	-6.103519	0.683487	-1.638312
6	-6.228794	0.843077	0.849472
6	1.577019	-3.791023	2.692570

6	-0.360358	-3.260437	4.054772
1	-2.162283	-2.814259	2.936889
6	2.468902	-3.474122	-0.492397
6	1.467130	-2.597983	-2.527807
1	-0.696025	-2.426069	-2.471766
1	-5.125521	-4.126764	1.517068
1	-4.186934	-5.633554	1.350598
1	-3.490363	-4.246075	2.214544
1	-5.436413	-4.283899	-1.003735
1	-4.323300	-5.661776	-1.163876
1	-4.025891	-4.161353	-2.085281
6	-0.561584	3.152137	-3.017270
6	-2.057023	1.737043	-4.307329
1	-3.508199	0.642843	-3.130494
6	-0.025430	3.971883	0.137794
6	-0.976103	3.535807	2.334250
1	-2.768551	2.312755	2.320058
1	-6.641926	-0.276422	-1.645341
1	-6.847055	1.491676	-1.712561
1	-5.470130	0.726409	-2.534372
1	-6.827064	-0.080258	0.883103
1	-6.922289	1.696272	0.790812
1	-5.663861	0.917232	1.790427
6	0.993660	-3.642650	3.964161

1	2.643939	-4.010448	2.614235
6	-1.068384	-2.973954	5.383407
6	2.609877	-3.017488	-1.814509
1	3.357393	-3.754469	0.078622
6	1.521305	-1.921716	-3.901841
6	-0.954505	2.618461	-4.257014
1	0.285233	3.839742	-2.968590
6	-2.611141	1.153871	-5.614511
6	0.037958	4.112261	1.533468
1	0.749883	4.417032	-0.487679
6	-1.032074	3.756927	3.851925
6	1.877546	-3.843518	5.199806
6	-0.060671	-2.916828	6.542512
6	-1.781993	-1.614006	5.319215
6	-2.108167	-4.075474	5.649213
6	4.017649	-2.893293	-2.400650
6	0.814573	-2.808905	-4.939409
6	2.971583	-1.661114	-4.349221
6	0.806413	-0.562286	-3.820540
6	-0.185538	3.052783	-5.509634
6	-2.003668	1.874757	-6.828631
6	-2.303547	-0.350895	-5.695461
6	-4.136097	1.340609	-5.673889
6	1.282396	4.786299	2.122133

6	0.365586	4.100401	4.388034
6	-2.011078	4.912096	4.130055
6	-1.517889	2.517906	4.614903
6	0.997826	-4.000947	6.448465
6	2.733283	-5.110840	5.063922
6	2.813163	-2.633273	5.356963
1	-0.612337	-2.989969	7.493460
1	0.427692	-1.929147	6.545223
1	-1.074334	-0.825648	5.019663
1	-2.187205	-1.357865	6.310604
1	-2.619949	-1.612677	4.607503
1	-2.828374	-4.143363	4.820401
1	-2.667744	-3.858945	6.572516
1	-1.630426	-5.060112	5.754867
6	3.924452	-2.765306	-3.927897
6	4.690104	-1.651173	-1.788371
6	4.873593	-4.126374	-2.082651
1	-0.220555	-3.026677	-4.638282
1	0.785296	-2.301739	-5.916845
1	1.336639	-3.769382	-5.063097
1	3.316925	-0.705213	-3.925229
1	2.985685	-1.530346	-5.443057
1	1.264997	0.076276	-3.048973
1	0.885943	-0.042514	-4.789096

1	-0.263312	-0.653348	-3.582197
6	-0.511186	2.110570	-6.677948
6	1.332625	3.011407	-5.278122
6	-0.581776	4.497179	-5.862417
1	-2.515345	2.840869	-6.967090
1	-2.214943	1.282380	-7.733097
1	-2.673976	-0.876310	-4.801630
1	-2.794901	-0.789143	-6.578166
1	-1.224596	-0.542648	-5.769644
1	-4.409949	2.391558	-5.498557
1	-4.506065	1.047824	-6.668797
1	-4.659246	0.720395	-4.932214
6	1.050986	5.189981	3.584882
6	1.676047	6.050635	1.346270
6	2.434576	3.767838	2.030123
1	0.276773	4.397808	5.445382
1	0.981719	3.185283	4.371540
1	-3.017644	4.653261	3.769910
1	-2.070451	5.113508	5.211517
1	-1.706725	5.835211	3.617617
1	-0.869819	1.652844	4.412858
1	-1.481293	2.720071	5.696446
1	-2.554539	2.245562	4.371496
1	1.643545	-3.988746	7.341272

1	0.515596	-4.992945	6.423924
1	2.107287	-5.988714	4.845989
1	3.270606	-5.294749	6.007134
1	3.487618	-5.019471	4.270003
1	3.456420	-2.516826	4.471415
1	3.459770	-2.761280	6.240433
1	2.251402	-1.695358	5.467138
1	4.931975	-2.581773	-4.334791
1	3.586846	-3.731002	-4.342138
1	4.810936	-1.778003	-0.702096
1	5.686360	-1.488080	-2.229788
1	4.086282	-0.744748	-1.935534
1	4.380705	-5.048000	-2.425414
1	5.844388	-4.042441	-2.595018
1	5.079931	-4.226678	-1.007878
1	-0.088408	2.532442	-7.603822
1	0.001130	1.147205	-6.513069
1	1.651453	2.026649	-4.907805
1	1.853818	3.209386	-6.227494
1	1.665673	3.771321	-4.557792
1	-0.333661	5.175833	-5.033102
1	-0.037563	4.835673	-6.758319
1	-1.660125	4.591304	-6.052153
1	2.022517	5.447328	4.036678

1	0.444308	6.109828	3.613705
1	0.830934	6.751452	1.277304
1	2.502503	6.556902	1.868466
1	2.024023	5.828336	0.328359
1	2.629754	3.501085	0.980838
1	3.359021	4.185052	2.460484
1	2.192033	2.833796	2.555996
1	-1.027485	0.328737	2.689353
6	2.473157	-0.304698	2.705999
6	3.076195	0.472378	3.717934
6	3.300905	-1.183901	1.974567
6	4.434462	0.351760	3.995174
1	2.462026	1.160179	4.301277
6	4.648335	-1.294051	2.271714
1	2.862937	-1.745578	1.152599
6	5.254883	-0.536486	3.289250
1	4.852104	0.969858	4.789658
1	5.253038	-1.985397	1.678433
6	6.753425	-0.685506	3.556948
6	7.208460	0.171256	4.741423
1	8.284992	0.024681	4.911617
1	7.041769	1.241924	4.552284
1	6.679183	-0.105122	5.665410
6	7.078174	-2.156610	3.866082

1	6.814614	-2.815604	3.026321
1	8.155776	-2.274098	4.059173
1	6.526388	-2.500835	4.753740
6	7.532468	-0.241563	2.306820
1	7.317647	0.811096	2.070803
1	8.615774	-0.347162	2.474378
1	7.263327	-0.845770	1.428286

Table S25

[Sb-T/S]

E : -3499.395829 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
51	-0.019747	0.122331	0.082644
6	-0.023495	0.258827	2.293554
6	1.174937	-0.142325	2.473352
6	-2.039095	-0.794365	0.070203
6	-2.308256	-2.164204	0.218091
6	-3.162508	0.052426	-0.065675
6	-1.314912	-3.304436	0.395426
6	-3.618852	-2.668718	0.233434

6	-3.198325	1.546398	-0.423005
6	-4.470355	-0.448947	-0.016341
6	-2.188015	-4.564681	0.093796
6	-0.661256	-3.351547	1.774192
6	-0.088978	-3.286078	-0.496971
6	-3.669223	-4.184301	0.327249
6	-4.709222	-1.812957	0.136301
6	-4.699801	1.924656	-0.244433
6	-2.667053	1.764758	-1.839132
6	-2.293741	2.477549	0.372755
6	-5.535529	0.621699	-0.165473
1	-1.867965	-5.432510	0.687716
1	-2.049991	-4.820446	-0.967767
6	0.710102	-3.642375	1.660238
6	-1.202552	-3.095875	3.018161
6	1.070411	-3.585662	0.233095
6	-0.006193	-2.952193	-1.833864
6	-4.180897	-4.651392	1.696933
6	-4.565051	-4.776729	-0.766292
1	-5.731234	-2.202732	0.157383
1	-5.036695	2.588981	-1.053051
1	-4.806113	2.484471	0.695686
6	-1.640846	2.723342	-1.851019
6	-3.046203	1.153581	-3.020362

6	-1.403205	3.160333	-0.467600
6	-2.256103	2.693677	1.740647
6	-6.386174	0.404967	-1.423420
6	-6.456659	0.638181	1.061128
6	1.484779	-3.779678	2.803196
6	-0.418623	-3.183137	4.186040
1	-2.245363	-2.778598	3.090857
6	2.298268	-3.602817	-0.414426
6	1.243632	-2.842739	-2.469993
1	-0.919701	-2.678285	-2.369742
1	-5.184461	-4.245040	1.895638
1	-4.244532	-5.749939	1.722936
1	-3.513278	-4.334200	2.507974
1	-5.620354	-4.509823	-0.603298
1	-4.493664	-5.875407	-0.766803
1	-4.266983	-4.408914	-1.759122
6	-0.999960	3.036924	-3.041117
6	-2.452520	1.506759	-4.247772
1	-3.818981	0.381976	-2.999991
6	-0.409581	3.956951	0.080146
6	-1.260503	3.503889	2.314026
1	-2.984117	2.187456	2.379377
1	-6.893304	-0.571091	-1.391787
1	-7.157094	1.186923	-1.501598

1	-5.774810	0.443918	-2.334977
1	-7.035810	-0.294983	1.134609
1	-7.168862	1.475188	0.994975
1	-5.871556	0.750542	1.985959
6	0.930855	-3.578360	4.080786
1	2.547967	-4.011364	2.710293
6	-1.094877	-2.839179	5.518274
6	2.405010	-3.218505	-1.762424
1	3.201041	-3.854674	0.146459
6	1.264356	-2.244660	-3.881102
6	-1.389223	2.435781	-4.251476
1	-0.183234	3.761596	-3.036057
6	-3.020304	0.870064	-5.523693
6	-0.292679	4.102394	1.470883
1	0.326989	4.421282	-0.577224
6	-1.290881	3.788400	3.820543
6	1.837866	-3.747934	5.304440
6	-0.063295	-2.759934	6.655102
6	-1.786132	-1.470063	5.421379
6	-2.146834	-3.913014	5.843245
6	3.797751	-3.134511	-2.389960
6	0.530490	-3.186615	-4.849250
6	2.703755	-2.012775	-4.377643
6	0.556190	-0.878814	-3.860985

6	-0.645032	2.835887	-5.529922
6	-2.461171	1.573585	-6.770379
6	-2.677019	-0.627928	-5.571685
6	-4.550386	1.018640	-5.547844
6	0.969971	4.783305	2.013357
6	0.125164	4.113163	4.317757
6	-2.232376	4.986608	4.047079
6	-1.812705	2.609222	4.649121
6	0.978927	-3.860416	6.572145
6	2.678542	-5.027916	5.193025
6	2.789060	-2.543790	5.408225
1	-0.595505	-2.796916	7.619131
1	0.438814	-1.779921	6.618465
1	-1.063852	-0.702881	5.103475
1	-2.184985	-1.181602	6.406552
1	-2.624188	-1.470969	4.709554
1	-2.887074	-3.996521	5.033779
1	-2.681938	-3.656466	6.770821
1	-1.683281	-4.901794	5.971589
6	3.665993	-3.093131	-3.919062
6	4.494299	-1.866357	-1.864628
6	4.655182	-4.353998	-2.025696
1	-0.495463	-3.388392	-4.508339
1	0.473726	-2.734472	-5.851873

1	1.050898	-4.152194	-4.933965
1	3.060476	-1.035975	-4.014719
1	2.691651	-1.941951	-5.476880
1	1.042801	-0.200072	-3.142776
1	0.612335	-0.415985	-4.859996
1	-0.506501	-0.951625	-3.586435
6	-0.972328	1.848477	-6.659593
6	0.875491	2.812389	-5.311605
6	-1.058438	4.262147	-5.930757
1	-2.999502	2.523775	-6.919547
1	-2.679455	0.953826	-7.654671
1	-3.011413	-1.138446	-4.655287
1	-3.178876	-1.102559	-6.429119
1	-1.595809	-0.794216	-5.669348
1	-4.844244	2.068652	-5.401657
1	-4.940090	0.681694	-6.521059
1	-5.037451	0.414322	-4.769328
6	0.800831	5.187908	3.485202
6	1.337784	6.044642	1.221105
6	2.115814	3.760395	1.881630
1	0.070513	4.424130	5.373613
1	0.724289	3.186489	4.293050
1	-3.254618	4.727243	3.734255
1	-2.255304	5.264471	5.113023

1	-1.924621	5.863956	3.461816
1	-1.194086	1.713209	4.498510
1	-1.767206	2.869146	5.717556
1	-2.858016	2.358326	4.421582
1	1.640400	-3.835246	7.453120
1	0.482890	-4.845858	6.580443
1	2.040015	-5.905850	5.015151
1	3.231251	-5.187164	6.131941
1	3.419063	-4.970172	4.383058
1	3.431221	-2.472506	4.517035
1	3.437600	-2.644450	6.293652
1	2.239878	-1.594687	5.481723
1	4.663076	-2.934792	-4.360369
1	3.317859	-4.080346	-4.268615
1	4.634052	-1.929743	-0.775055
1	5.483804	-1.742751	-2.332806
1	3.898551	-0.962672	-2.054419
1	4.144775	-5.289764	-2.296534
1	5.608643	-4.308963	-2.574023
1	4.896537	-4.391171	-0.954255
1	-0.577675	2.249150	-7.607104
1	-0.434608	0.903179	-6.473474
1	1.200283	1.842371	-4.908179
1	1.387684	2.977180	-6.272219

1	1.210519	3.599374	-4.621832
1	-0.819719	4.972280	-5.125487
1	-0.517488	4.576195	-6.837310
1	-2.137595	4.335664	-6.125064
1	1.793787	5.427520	3.898541
1	0.214092	6.119098	3.539517
1	0.492421	6.747544	1.181704
1	2.183338	6.550645	1.711806
1	1.648231	5.819305	0.191676
1	2.268730	3.488651	0.826318
1	3.057088	4.178210	2.273380
1	1.889500	2.829458	2.421532
1	-0.936519	0.405896	2.877836
6	2.561616	-0.320331	2.698302
6	3.217323	0.512744	3.628561
6	3.343536	-1.261619	1.995483
6	4.584144	0.389620	3.857313
1	2.637523	1.251637	4.184140
6	4.701596	-1.372853	2.241773
1	2.863346	-1.869576	1.230390
6	5.362288	-0.554282	3.176574
1	5.043395	1.057539	4.585862
1	5.273377	-2.107930	1.668830
6	6.872374	-0.693153	3.376516

6	7.391983	0.240321	4.473439
1	8.476099	0.097773	4.595093
1	7.220258	1.296564	4.219212
1	6.910668	0.033248	5.440703
6	7.211140	-2.140716	3.767737
1	6.904433	-2.855145	2.990352
1	8.297062	-2.249437	3.913923
1	6.704909	-2.419957	4.703821
6	7.583930	-0.336695	2.060424
1	7.353096	0.697311	1.765508
1	8.674910	-0.427824	2.178204
1	7.273457	-0.999651	1.239933

Table S26

[Bi-T/S]

E : -3473.713174 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
83	0.003531	-0.068815	0.169810
6	-0.202898	0.089618	2.384723
6	0.728499	0.219312	3.356346

6	-2.137009	-0.864922	0.054984
6	-2.420567	-2.210132	0.292949
6	-3.242052	-0.036513	-0.134493
6	-1.413419	-3.313441	0.530799
6	-3.730583	-2.708155	0.308448
6	-3.186243	1.420430	-0.561262
6	-4.558324	-0.488846	-0.032869
6	-2.258671	-4.591348	0.235019
6	-0.773248	-3.300527	1.918331
6	-0.181457	-3.199738	-0.346265
6	-3.754839	-4.224657	0.442584
6	-4.817710	-1.844067	0.180254
6	-4.654593	1.897015	-0.396480
6	-2.621450	1.508658	-1.977380
6	-2.130223	2.176464	0.227773
6	-5.561173	0.644925	-0.172359
1	-1.940013	-5.443477	0.851966
1	-2.102003	-4.863569	-0.819889
6	0.618362	-3.474452	1.824680
6	-1.345062	-3.049185	3.149966
6	0.996892	-3.391305	0.400611
6	-0.112077	-2.900480	-1.696372
6	-4.275572	-4.671874	1.815771
6	-4.627655	-4.857246	-0.647260

1	-5.843726	-2.220375	0.227661
1	-4.974616	2.479251	-1.272115
1	-4.720018	2.566864	0.473081
6	-1.368186	2.133802	-1.987124
6	-3.155407	1.040924	-3.164907
6	-1.026234	2.488937	-0.595553
6	-2.133266	2.570875	1.556204
6	-6.525366	0.413924	-1.341597
6	-6.366672	0.791842	1.125573
6	1.394391	-3.513287	2.973321
6	-0.559734	-2.998978	4.315139
1	-2.405225	-2.796755	3.209385
6	2.225312	-3.360326	-0.251913
6	1.127798	-2.809211	-2.355890
1	-1.039205	-2.700571	-2.241030
1	-5.290050	-4.282393	1.990416
1	-4.316065	-5.770779	1.865849
1	-3.627906	-4.322624	2.629070
1	-5.688450	-4.600733	-0.503770
1	-4.541672	-5.954163	-0.617005
1	-4.323918	-4.512926	-1.646713
6	-0.707052	2.364425	-3.186287
6	-2.504754	1.259425	-4.392203
1	-4.100360	0.496172	-3.145608

6	0.061330	3.187245	-0.056269
6	-1.054512	3.284969	2.101925
1	-2.980727	2.308034	2.191783
1	-7.111182	-0.504930	-1.188296
1	-7.229550	1.255047	-1.432049
1	-5.987447	0.315471	-2.295177
1	-6.974175	-0.105521	1.316381
1	-7.044284	1.657226	1.062617
1	-5.694898	0.935108	1.984963
6	0.817662	-3.295529	4.235022
1	2.475546	-3.647393	2.895035
6	-1.248923	-2.570043	5.612911
6	2.305529	-3.094917	-1.633523
1	3.140315	-3.521955	0.321389
6	1.109462	-2.353990	-3.818213
6	-1.275018	1.959078	-4.404343
1	0.251997	2.884932	-3.180484
6	-3.146451	0.668799	-5.654943
6	0.048170	3.623059	1.274084
1	0.902727	3.442988	-0.703848
6	-1.114594	3.708280	3.569135
6	1.731903	-3.340025	5.463191
6	-0.207621	-2.302879	6.710369
6	-2.010906	-1.254495	5.381692

6	-2.226977	-3.669061	6.057864
6	3.682756	-3.081539	-2.301926
6	0.379494	-3.400557	-4.676186
6	2.535601	-2.148351	-4.357302
6	0.371382	-1.010804	-3.918941
6	-0.593064	2.375551	-5.710588
6	-2.535537	1.280032	-6.926302
6	-2.914899	-0.853709	-5.652151
6	-4.659533	0.931303	-5.689280
6	1.248940	4.452260	1.744293
6	0.312787	3.980085	4.065442
6	-1.992691	4.969587	3.664943
6	-1.707432	2.609637	4.462377
6	0.881580	-3.359864	6.741376
6	2.589814	-4.613525	5.443231
6	2.658821	-2.112996	5.460630
1	-0.726252	-2.243614	7.680857
1	0.241642	-1.314083	6.524913
1	-1.321708	-0.510344	4.950113
1	-2.389559	-0.877908	6.345485
1	-2.875750	-1.381076	4.713677
1	-2.965544	-3.879341	5.269101
1	-2.772628	-3.350116	6.959641
1	-1.704238	-4.610640	6.282079

6	3.512023	-3.181764	-3.825206
6	4.417538	-1.784798	-1.924850
6	4.527718	-4.278019	-1.840940
1	-0.644859	-3.572024	-4.314429
1	0.316810	-3.055760	-5.720226
1	0.905822	-4.366235	-4.662079
1	2.886072	-1.140848	-4.082860
1	2.505095	-2.168993	-5.458043
1	0.866043	-0.244547	-3.301206
1	0.378520	-0.662236	-4.964092
1	-0.679163	-1.066305	-3.594832
6	-1.026332	1.436488	-6.845794
6	0.938127	2.338768	-5.611408
6	-1.018878	3.823970	-6.019428
1	-2.996980	2.263151	-7.111579
1	-2.810682	0.646833	-7.784901
1	-3.296568	-1.306243	-4.724060
1	-3.439208	-1.318124	-6.501461
1	-1.846879	-1.100587	-5.728116
1	-4.877175	2.001740	-5.558582
1	-5.063415	0.612641	-6.662494
1	-5.199875	0.370807	-4.913272
6	1.049332	4.968919	3.180602
6	1.435750	5.668725	0.823069

6	2.507557	3.573674	1.685001
1	0.261006	4.356626	5.099068
1	0.842299	3.012150	4.101198
1	-3.029717	4.734665	3.380865
1	-1.998719	5.346832	4.699267
1	-1.643482	5.773992	3.001718
1	-1.104415	1.691262	4.382017
1	-1.675454	2.953372	5.507780
1	-2.760290	2.393841	4.228758
1	1.545179	-3.213545	7.608830
1	0.429056	-4.360250	6.856738
1	1.963061	-5.511432	5.333083
1	3.148453	-4.693850	6.388830
1	3.325089	-4.603128	4.625825
1	3.291616	-2.097562	4.558333
1	3.319564	-2.140273	6.342343
1	2.084805	-1.175854	5.458992
1	4.498312	-3.064609	-4.301689
1	3.157035	-4.196053	-4.076432
1	4.555232	-1.722854	-0.836795
1	5.410685	-1.753294	-2.400154
1	3.856271	-0.889268	-2.225811
1	3.988743	-5.224535	-1.993080
1	5.460486	-4.315605	-2.423778

1	4.808283	-4.207723	-0.780800
1	-0.632309	1.825180	-7.798263
1	-0.553342	0.451380	-6.692114
1	1.295716	1.363409	-5.251755
1	1.372607	2.519295	-6.606152
1	1.331382	3.117684	-4.943063
1	-0.678734	4.497016	-5.218381
1	-0.573296	4.161266	-6.968777
1	-2.110796	3.924882	-6.088516
1	2.038901	5.205484	3.601723
1	0.494273	5.920653	3.153495
1	0.511579	6.263366	0.762782
1	2.232883	6.311964	1.225833
1	1.727343	5.379617	-0.196928
1	2.674518	3.172119	0.673415
1	3.394372	4.162771	1.965183
1	2.427274	2.721179	2.370034
1	-1.281266	0.000744	2.595015
6	2.148785	0.119669	3.020624
6	3.088713	0.852079	3.782216
6	2.708017	-0.780007	2.085786
6	4.459924	0.710609	3.620333
1	2.699068	1.522740	4.552248
6	4.085322	-0.955216	1.953264

1	2.050579	-1.447503	1.533490
6	4.998237	-0.226112	2.720588
1	5.121404	1.306753	4.249589
1	4.453722	-1.719791	1.263668
6	6.495048	-0.529469	2.618621
6	7.330401	0.415011	3.486966
1	8.398086	0.176586	3.372533
1	7.181706	1.465533	3.196222
1	7.076646	0.312699	4.552167
6	6.743592	-1.970915	3.096161
1	6.198395	-2.697065	2.474781
1	7.816417	-2.215884	3.046299
1	6.404772	-2.095730	4.135738
6	6.956871	-0.387142	1.160020
1	6.771392	0.633432	0.793336
1	8.034205	-0.598868	1.074519
1	6.424640	-1.085793	0.498262

Table S27

[N-Prod]¹

E : -3313.92433896 Hartree

G : -3312.37832450 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	0.029979	0.153132	-0.093974
6	-0.024875	0.161575	1.319714
6	1.174960	0.146891	2.056595
6	2.422820	0.064467	1.447347
1	3.334786	0.032264	2.049766
6	2.475010	-0.002440	0.059506
6	1.300925	0.057373	-0.691171
6	-0.554024	-0.028704	3.676918
1	-1.034357	0.571710	4.462808
1	-0.710825	-1.086208	3.932004
6	0.958757	0.230981	3.556765
6	1.355881	1.614939	4.090400
1	1.213000	1.656557	5.181322
1	2.414200	1.825072	3.873320
1	0.748596	2.410683	3.640412
6	1.756944	-0.840064	4.307978
1	1.484505	-0.840637	5.374689
1	1.555091	-1.840259	3.896992
1	2.839216	-0.652763	4.240004
6	3.117039	-0.347561	-2.219202
1	3.175740	-1.406483	-2.509024

1	3.666513	0.225855	-2.979517
6	3.715807	-0.173704	-0.798175
6	4.649935	1.039132	-0.698190
1	5.553300	0.874393	-1.305307
1	4.165356	1.955172	-1.060068
1	4.964049	1.204941	0.343627
6	4.488609	-1.430366	-0.377190
1	5.328717	-1.612645	-1.065149
1	4.899292	-1.321891	0.638285
1	3.832453	-2.313256	-0.388478
6	-1.218787	0.233681	2.276891
6	-1.987537	1.551088	2.281314
6	-1.518765	2.850513	2.239335
1	-0.457474	3.029890	2.055421
6	-2.389284	3.942302	2.417694
6	-3.769208	3.702300	2.600061
6	-4.240534	2.379224	2.579379
1	-5.307887	2.181810	2.696401
6	-3.365762	1.315386	2.411881
6	-3.598379	-0.129669	2.301420
6	-4.766682	-0.877983	2.288316
1	-5.727777	-0.372689	2.401021
6	-4.728403	-2.273803	2.129627
6	-3.477717	-2.915046	1.970527

6	-2.301544	-2.141630	2.002395
1	-1.327020	-2.625433	1.894984
6	-2.358113	-0.767263	2.144165
6	-1.783535	5.348747	2.360691
6	-0.500489	5.436167	3.200579
1	-0.161952	6.482849	3.246215
1	-0.675917	5.085134	4.228736
1	0.321166	4.846149	2.770248
6	-1.440146	5.662522	0.896368
1	-2.339706	5.656170	0.265412
1	-0.951957	6.647848	0.814407
1	-0.760435	4.902618	0.484191
6	-2.773256	6.391627	2.900322
1	-2.767846	6.361453	4.002289
1	-2.414475	7.394593	2.617930
6	-4.772949	4.830105	2.859593
6	-5.085789	4.874838	4.365341
1	-5.521785	3.919586	4.693367
1	-4.180935	5.045404	4.964998
1	-5.807697	5.677668	4.584138
6	-6.085879	4.606518	2.096352
1	-5.887819	4.428389	1.029453
1	-6.662970	3.757638	2.488721
1	-6.720522	5.501700	2.185856

6	-4.185197	6.167393	2.389837
1	-4.186895	6.178004	1.287426
1	-4.850347	6.984049	2.714425
6	-3.334783	-4.433214	1.812581
6	1.607999	0.064636	-2.182359
6	1.356848	1.424850	-2.826217
6	1.805903	2.673430	-2.437676
1	2.352501	2.776236	-1.498150
6	1.559913	3.815518	-3.225304
6	0.792724	3.681717	-4.403234
6	0.300940	2.413715	-4.761231
1	-0.302543	2.303415	-5.663902
6	0.584173	1.294473	-3.991339
6	0.214216	-0.118855	-4.144634
6	-0.552100	-0.772776	-5.096520
1	-0.997649	-0.200357	-5.912668
6	-0.762737	-2.160577	-5.022667
6	-0.149957	-2.892582	-3.982580
6	0.603283	-2.206352	-3.010686
1	1.055825	-2.760036	-2.183496
6	0.776881	-0.838611	-3.080843
6	2.129016	5.153722	-2.736392
6	3.604335	5.003041	-2.333072
1	4.031014	5.994884	-2.117178

1	3.728421	4.389313	-1.429664
1	4.188805	4.544107	-3.144360
6	1.335561	5.619663	-1.504069
1	0.280721	5.818027	-1.743125
1	1.353084	4.849265	-0.718283
1	1.775423	6.541190	-1.090841
6	2.054464	6.216765	-3.843687
1	2.216991	7.208213	-3.391291
1	2.887289	6.060885	-4.548208
6	0.521597	4.859523	-5.344844
6	-0.918015	4.835132	-5.881973
1	-1.073391	4.028709	-6.612087
1	-1.647686	4.697665	-5.070315
1	-1.137567	5.784982	-6.394335
6	1.482525	4.759703	-6.543447
1	1.321163	3.814582	-7.082330
1	1.309088	5.591542	-7.244555
1	2.534714	4.781224	-6.227845
6	0.738598	6.185888	-4.601184
1	0.692262	7.013002	-5.328010
1	-0.096061	6.348504	-3.898884
6	-1.630047	-2.816962	-6.103190
6	-2.923127	-2.018841	-6.328830
1	-3.458826	-1.865378	-5.380499

1	-2.734006	-1.033969	-6.777671
1	-3.583465	-2.572184	-7.014644
6	-0.843374	-2.862319	-7.424137
1	-0.557189	-1.847361	-7.736844
1	0.081224	-3.448490	-7.326331
1	-1.457498	-3.308121	-8.222565
6	-2.030323	-4.236334	-5.674400
1	-2.819235	-4.166809	-4.906916
1	-2.480667	-4.754319	-6.536483
6	-0.285172	-4.412645	-3.840926
6	-1.206514	-4.717241	-2.649322
1	-2.212890	-4.299292	-2.798941
1	-1.298795	-5.804489	-2.495632
1	-0.799091	-4.273604	-1.729605
6	1.081990	-5.063755	-3.581029
1	0.977514	-6.159868	-3.597247
1	1.806660	-4.774622	-4.356455
1	1.497516	-4.786676	-2.602285
6	-0.856465	-5.027370	-5.126932
1	-0.058029	-5.075467	-5.885732
1	-1.150503	-6.069260	-4.921117
6	-2.788299	-5.017311	3.126808
1	-3.469180	-4.827141	3.968600
1	-2.645267	-6.105052	3.031519

1	-1.818049	-4.563997	3.377746
6	-2.364144	-4.775727	0.674709
1	-2.673044	-4.283995	-0.259015
1	-1.330502	-4.474204	0.894955
1	-2.360760	-5.863436	0.502290
6	-4.688589	-5.073802	1.472113
1	-4.911671	-4.893823	0.407567
1	-4.600984	-6.165932	1.587703
6	-6.059568	-3.033977	2.103029
6	-7.003912	-2.545056	3.211372
1	-7.358433	-1.519406	3.039709
1	-7.891282	-3.195403	3.249979
1	-6.508792	-2.578840	4.192986
6	-6.736944	-2.798176	0.741761
1	-6.112704	-3.153295	-0.090379
1	-7.705895	-3.319994	0.698579
1	-6.916966	-1.724600	0.583119
6	-5.820054	-4.534138	2.327016
1	-5.592940	-4.702789	3.392850
6	-2.395087	-0.219865	-0.620699
1	-2.946224	-1.146760	-0.513911
6	-2.235638	1.045149	-0.795800
6	-2.624663	2.391173	-1.134672
6	-3.923139	2.858120	-0.870605

1	-4.619416	2.225266	-0.317144
6	-4.317643	4.106520	-1.330809
1	-5.340454	4.437359	-1.138358
6	-3.445476	4.937769	-2.056420
6	-2.153625	4.459737	-2.297649
1	-1.437518	5.057202	-2.860223
6	-1.738802	3.208424	-1.842003
1	-0.732613	2.846461	-2.057982
6	-3.938287	6.295073	-2.567163
6	-5.028799	6.055252	-3.624677
1	-4.630936	5.465263	-4.463763
1	-5.398545	7.014777	-4.018166
1	-5.883046	5.507654	-3.200533
6	-4.521531	7.117654	-1.407165
1	-5.346751	6.595246	-0.901734
1	-4.911992	8.075318	-1.783939
1	-3.746183	7.337090	-0.657502
6	-2.808296	7.110340	-3.202100
1	-1.982006	7.269899	-2.491360
1	-3.188942	8.096252	-3.506799
1	-2.403733	6.617526	-4.097498
7	-1.040911	0.185269	-1.052992
1	-6.755940	-5.077279	2.119382

Table S28**[P-Prod]¹**

E : -3600.52190990 Hartree

G : -3598.96446009 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	-0.026288	0.009254	-0.040151
6	-0.072085	0.041787	1.372510
6	1.115247	0.116491	2.125528
6	2.363917	0.145680	1.517722
1	3.275865	0.186013	2.120393
6	2.429029	0.091846	0.131644
6	1.259148	0.030894	-0.637327
6	-0.600595	-0.245483	3.712670
1	-1.130006	0.249475	4.539666
1	-0.683587	-1.331138	3.868469
6	0.889695	0.126887	3.626478
6	1.192341	1.503375	4.235889
1	1.054433	1.470858	5.327674
1	2.233836	1.795545	4.031284
1	0.531085	2.281991	3.836316

6	1.754709	-0.925470	4.329725
1	1.473720	-1.000434	5.391596
1	1.626154	-1.914150	3.865272
1	2.821898	-0.660164	4.284694
6	3.169641	-0.192378	-2.117145
1	3.330053	-1.245410	-2.388349
1	3.683888	0.418103	-2.873166
6	3.705414	0.049297	-0.686933
6	4.506158	1.352433	-0.567071
1	5.441184	1.277776	-1.143261
1	3.943560	2.212174	-0.951992
1	4.767563	1.554559	0.482870
6	4.594056	-1.118358	-0.237884
1	5.463412	-1.216228	-0.906349
1	4.969990	-0.961712	0.784640
1	4.033638	-2.064738	-0.255672
6	-1.266828	0.085373	2.330919
6	-1.992631	1.426797	2.402570
6	-1.500076	2.712431	2.303256
1	-0.450316	2.862424	2.041410
6	-2.334170	3.828251	2.513604
6	-3.703260	3.624528	2.787396
6	-4.203121	2.311081	2.832804
1	-5.266233	2.140623	3.012673

6	-3.364256	1.225128	2.632059
6	-3.643582	-0.210802	2.497249
6	-4.834988	-0.920416	2.500158
1	-5.768530	-0.402211	2.728789
6	-4.860274	-2.286813	2.167609
6	-3.651168	-2.936929	1.830769
6	-2.444341	-2.213598	1.883470
1	-1.500300	-2.705962	1.637225
6	-2.439734	-0.867792	2.191245
6	-1.700470	5.215784	2.371373
6	-0.384425	5.304755	3.158484
1	-0.012562	6.340961	3.137902
1	-0.531838	5.012116	4.209197
1	0.401596	4.666369	2.730300
6	-1.407764	5.452337	0.882229
1	-2.333662	5.464465	0.291090
1	-0.879027	6.409072	0.736490
1	-0.782768	4.644802	0.474962
6	-2.641828	6.309761	2.896523
1	-2.577592	6.350345	3.996177
1	-2.282391	7.285732	2.531721
6	-4.664344	4.786145	3.058376
6	-4.869275	4.914112	4.577741
1	-5.308398	3.989705	4.981403

1	-3.920234	5.083046	5.104933
1	-5.550874	5.749076	4.805716
6	-6.033331	4.556341	2.403010
1	-5.920393	4.321744	1.334520
1	-6.597110	3.741775	2.878441
1	-6.641750	5.469427	2.493200
6	-4.082870	6.082168	2.476707
1	-4.141935	6.025940	1.376607
1	-4.716240	6.929716	2.785758
6	-3.584890	-4.412138	1.423527
6	1.628956	0.081317	-2.129248
6	1.297897	1.418666	-2.794019
6	1.621353	2.703820	-2.396786
1	2.084097	2.861978	-1.420591
6	1.385724	3.809729	-3.238792
6	0.714315	3.606957	-4.464444
6	0.341267	2.301735	-4.832527
1	-0.174138	2.134276	-5.780201
6	0.648542	1.216304	-4.024053
6	0.422834	-0.224831	-4.198186
6	-0.231033	-0.942399	-5.187116
1	-0.662175	-0.413004	-6.039087
6	-0.359345	-2.339039	-5.097699
6	0.230121	-3.015632	-4.006684

6	0.879837	-2.268811	-3.006906
1	1.305807	-2.777863	-2.138007
6	0.958429	-0.892629	-3.088276
6	1.900463	5.180089	-2.778467
6	3.360849	5.074479	-2.309590
1	3.760298	6.082454	-2.117707
1	3.456816	4.500844	-1.376886
1	3.987188	4.593993	-3.075974
6	1.053096	5.681031	-1.599574
1	-0.001688	5.822005	-1.875952
1	1.077763	4.956251	-0.772994
1	1.446587	6.639238	-1.224574
6	1.857192	6.192072	-3.934011
1	1.986120	7.204812	-3.519882
1	2.720900	6.018223	-4.596212
6	0.422686	4.747060	-5.446711
6	-1.006261	4.655645	-6.004285
1	-1.135300	3.797111	-6.677905
1	-1.747774	4.564155	-5.196984
1	-1.233398	5.563591	-6.584728
6	1.408062	4.648802	-6.625034
1	1.295111	3.683307	-7.139473
1	1.215169	5.452092	-7.353509
1	2.452507	4.722613	-6.291614

6	0.575602	6.103356	-4.742466
1	0.538114	6.902958	-5.499722
1	-0.290464	6.268877	-4.080276
6	-1.113975	-3.065060	-6.217386
6	-2.435017	-2.350861	-6.541247
1	-3.036441	-2.209950	-5.631210
1	-2.276854	-1.366452	-7.002971
1	-3.017246	-2.957743	-7.251938
6	-0.239561	-3.082606	-7.482766
1	0.008559	-2.057390	-7.794601
1	0.708042	-3.613357	-7.314190
1	-0.773326	-3.574630	-8.311102
6	-1.455651	-4.499967	-5.789300
1	-2.301663	-4.468921	-5.082984
1	-1.808514	-5.058106	-6.671414
6	0.158393	-4.536262	-3.832767
6	-0.842287	-4.855803	-2.709944
1	-1.851664	-4.492498	-2.949791
1	-0.892596	-5.942350	-2.534064
1	-0.535564	-4.368164	-1.773457
6	1.529353	-5.112324	-3.447903
1	1.478437	-6.212210	-3.443179
1	2.300270	-4.805928	-4.170364
1	1.850551	-4.794058	-2.446423

6	-0.279332	-5.207917	-5.142520
1	0.574260	-5.221412	-5.840429
1	-0.525911	-6.261562	-4.934604
6	-3.005114	-5.227856	2.591906
1	-3.635718	-5.158718	3.489488
1	-2.913789	-6.288406	2.309342
1	-2.005212	-4.857035	2.861498
6	-2.678962	-4.595194	0.197252
1	-2.965579	-3.905934	-0.611219
1	-1.620220	-4.419472	0.432734
1	-2.763730	-5.626578	-0.179689
6	-4.983087	-4.929616	1.055981
1	-5.253315	-4.547362	0.057681
1	-4.941944	-6.026948	0.966253
6	-6.221511	-2.990916	2.129867
6	-7.042959	-2.672297	3.387841
1	-7.345081	-1.616938	3.435196
1	-7.962194	-3.278165	3.390199
1	-6.472660	-2.907743	4.298431
6	-6.997982	-2.499842	0.895350
1	-6.462171	-2.727862	-0.037193
1	-7.990964	-2.974185	0.852116
1	-7.140125	-1.409745	0.935887
6	-6.037760	-4.514468	2.065712

1	-5.756721	-4.882657	3.066233
6	-3.042440	0.035932	-0.460178
1	-3.874260	-0.519340	-0.032867
6	-2.625498	1.192168	-0.906106
6	-2.934157	2.578031	-1.209972
6	-4.123264	3.177278	-0.762208
1	-4.789077	2.612266	-0.105899
6	-4.451242	4.465313	-1.164381
1	-5.390345	4.903930	-0.818622
6	-3.608941	5.209330	-2.010148
6	-2.420190	4.604937	-2.430780
1	-1.730354	5.136369	-3.083678
6	-2.080914	3.310412	-2.038786
1	-1.153552	2.851578	-2.392278
6	-4.012345	6.623278	-2.436190
6	-5.290777	6.542570	-3.286335
1	-5.119564	5.934927	-4.187140
1	-5.605116	7.549876	-3.600431
1	-6.118122	6.087542	-2.722748
6	-4.279064	7.483294	-1.189929
1	-5.105689	7.081981	-0.585755
1	-4.549915	8.507742	-1.487920
1	-3.383973	7.534893	-0.550909
6	-2.915400	7.301942	-3.261569

1	-1.976128	7.378829	-2.691670
1	-3.231131	8.320084	-3.532159
1	-2.709572	6.755256	-4.194096
15	-1.428525	-0.140558	-1.295960
1	-7.008442	-4.977879	1.827059

Table S29

[As-Prod]¹

E : -5494.89855181 Hartree

G : -5493.353589 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.044063	0.000245	-0.019738
6	-0.028938	-0.010219	1.393079
6	1.189032	0.047327	2.097779
6	2.406867	0.152743	1.437048
1	3.344050	0.197341	1.999419
6	2.409592	0.156949	0.048126
6	1.208860	0.059192	-0.669727
6	-0.458834	-0.443989	3.728247
1	-0.943840	-0.003948	4.611746

1	-0.554057	-1.536824	3.808865
6	1.033871	-0.082993	3.603172
6	1.398148	1.209232	4.347100
1	1.340121	1.045955	5.434267
1	2.426000	1.520103	4.104172
1	0.719007	2.032759	4.096829
6	1.911510	-1.220603	4.141191
1	1.685360	-1.406185	5.202648
1	1.736425	-2.150122	3.579948
1	2.980297	-0.969188	4.064491
6	3.055754	-0.123070	-2.220030
1	3.236511	-1.188512	-2.422514
1	3.514442	0.449172	-3.039268
6	3.641194	0.225990	-0.835157
6	4.276563	1.623148	-0.802260
1	5.184772	1.640506	-1.424270
1	3.591822	2.389621	-1.186507
1	4.559696	1.896430	0.225802
6	4.691238	-0.806855	-0.410442
1	5.518556	-0.830679	-1.136392
1	5.116891	-0.560497	0.574239
1	4.250821	-1.813137	-0.352458
6	-1.178302	-0.004963	2.407289
6	-1.842707	1.359977	2.589239

6	-1.288427	2.625410	2.596576
1	-0.225462	2.744673	2.374490
6	-2.072538	3.762771	2.879544
6	-3.463361	3.610156	3.062131
6	-4.019423	2.317991	3.033048
1	-5.095390	2.189731	3.168406
6	-3.222053	1.205313	2.812254
6	-3.561878	-0.213638	2.627373
6	-4.777886	-0.879885	2.661683
1	-5.681248	-0.335247	2.944327
6	-4.865002	-2.238730	2.311834
6	-3.694592	-2.922466	1.913698
6	-2.463268	-2.239357	1.919253
1	-1.548122	-2.762445	1.630005
6	-2.394919	-0.902189	2.257992
6	-1.354953	5.114534	2.976734
6	-0.155180	5.007540	3.931860
1	0.275952	6.007106	4.097604
1	-0.462588	4.597589	4.905643
1	0.641390	4.368083	3.525292
6	-0.835001	5.526303	1.591995
1	-1.647370	5.659853	0.862525
1	-0.268381	6.468589	1.660245
1	-0.162636	4.755114	1.190391

6	-2.301582	6.189794	3.530198
1	-2.380822	6.073978	4.623543
1	-1.852239	7.180277	3.355623
6	-4.405799	4.800666	3.272014
6	-4.872294	4.830204	4.736946
1	-5.396046	3.897309	4.992619
1	-4.027297	4.933585	5.431949
1	-5.565744	5.669682	4.902327
6	-5.641441	4.688727	2.365161
1	-5.349521	4.555570	1.312201
1	-6.294140	3.850956	2.646938
1	-6.238664	5.610542	2.442643
6	-3.684161	6.107378	2.911186
1	-3.597321	6.170967	1.812511
1	-4.308273	6.958953	3.225916
6	-3.695157	-4.397597	1.500874
6	1.503930	0.097007	-2.171899
6	1.109673	1.396175	-2.869364
6	1.263037	2.704543	-2.452308
1	1.587628	2.903246	-1.428782
6	1.001826	3.779682	-3.321901
6	0.540419	3.510044	-4.628961
6	0.303834	2.178533	-5.011510
1	-0.089256	1.959983	-6.005833

6	0.572534	1.131310	-4.139595
6	0.382877	-0.321390	-4.263248
6	-0.203067	-1.095579	-5.253592
1	-0.584380	-0.613784	-6.156029
6	-0.326100	-2.487357	-5.102289
6	0.194718	-3.102482	-3.941927
6	0.783008	-2.301287	-2.946211
1	1.163493	-2.761688	-2.030326
6	0.860040	-0.929963	-3.092792
6	1.185565	5.195081	-2.761656
6	2.542890	5.337612	-2.056279
1	2.700339	6.389203	-1.770217
1	2.599574	4.736898	-1.137267
1	3.367132	5.032908	-2.719074
6	0.065999	5.442716	-1.738394
1	-0.922018	5.444087	-2.218257
1	0.050669	4.647333	-0.980724
1	0.212710	6.408650	-1.227647
6	1.114607	6.258208	-3.869943
1	0.915833	7.236066	-3.401455
1	2.098249	6.349834	-4.357555
6	0.341890	4.629359	-5.654021
6	-0.828855	4.347114	-6.604795
1	-0.606945	3.531609	-7.307098

1	-1.739475	4.077777	-6.051230
1	-1.041442	5.244693	-7.205625
6	1.623520	4.744817	-6.499485
1	1.792296	3.811244	-7.056266
1	1.535150	5.569986	-7.224384
1	2.511610	4.918346	-5.876772
6	0.057764	5.945365	-4.914912
1	-0.013508	6.764580	-5.649452
1	-0.928797	5.862171	-4.427590
6	-0.996365	-3.278708	-6.231513
6	-2.286021	-2.588272	-6.700263
1	-2.956609	-2.392847	-5.850566
1	-2.089945	-1.634545	-7.209421
1	-2.812767	-3.239444	-7.414914
6	-0.025270	-3.369459	-7.421203
1	0.248004	-2.363847	-7.773315
1	0.905406	-3.886058	-7.147112
1	-0.493072	-3.912074	-8.257783
6	-1.374145	-4.686379	-5.746837
1	-2.268027	-4.614138	-5.105412
1	-1.666192	-5.294099	-6.618349
6	0.104272	-4.610079	-3.685985
6	-0.970956	-4.856595	-2.615033
1	-1.960495	-4.508451	-2.943988

1	-1.038350	-5.929139	-2.371774
1	-0.724417	-4.308019	-1.694761
6	1.442339	-5.166219	-3.176143
1	1.384460	-6.263952	-3.113872
1	2.262973	-4.902606	-3.859715
1	1.695902	-4.793703	-2.174033
6	-0.249521	-5.357444	-4.979604
1	0.648908	-5.416416	-5.616074
1	-0.517828	-6.395662	-4.726074
6	-3.103810	-5.236228	2.647361
1	-3.695888	-5.142899	3.568598
1	-3.064683	-6.299461	2.362636
1	-2.080566	-4.904717	2.877976
6	-2.839903	-4.612059	0.244422
1	-3.129249	-3.913357	-0.554820
1	-1.768229	-4.475477	0.444422
1	-2.973841	-5.639977	-0.127649
6	-5.123299	-4.862972	1.183000
1	-5.418442	-4.459154	0.200400
1	-5.123571	-5.959987	1.080267
6	-6.249960	-2.896250	2.327029
6	-7.004895	-2.565864	3.623122
1	-7.271142	-1.502147	3.693986
1	-7.942215	-3.142228	3.660005

1	-6.403368	-2.829304	4.505563
6	-7.062361	-2.364527	1.133170
1	-6.577053	-2.600641	0.175614
1	-8.072576	-2.803128	1.131068
1	-7.163412	-1.270657	1.189941
6	-6.122696	-4.424333	2.237998
1	-5.816837	-4.815666	3.222265
6	-3.099321	0.632229	-0.315737
1	-3.950673	0.458316	0.335387
6	-2.554500	1.501813	-1.118611
6	-2.760632	2.853300	-1.623057
6	-3.210305	3.849819	-0.741592
1	-3.275932	3.621874	0.326035
6	-3.566955	5.102772	-1.223905
1	-3.904177	5.862285	-0.513907
6	-3.516611	5.404240	-2.594819
6	-3.052856	4.404389	-3.456742
1	-3.000549	4.596293	-4.526796
6	-2.650441	3.155134	-2.982106
1	-2.274021	2.394758	-3.670996
6	-3.914639	6.800137	-3.083048
6	-5.315070	7.154525	-2.557451
1	-6.058763	6.423929	-2.908404
1	-5.612000	8.151585	-2.916744

1	-5.348273	7.172058	-1.459022
6	-2.892952	7.819207	-2.549524
1	-2.839298	7.794846	-1.450695
1	-3.172672	8.838652	-2.857533
1	-1.886422	7.604459	-2.940433
6	-3.940072	6.887960	-4.612403
1	-2.946369	6.708231	-5.048940
1	-4.259669	7.894859	-4.918171
1	-4.644427	6.161700	-5.044684
33	-1.623236	-0.236785	-1.232595
1	-7.117763	-4.850156	2.031871

Table S30

[Sb-Prod]¹

E : -3499.44168545 Hartree

G : -3497.897404 Hartree

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z
6	-0.014519	-0.019582	-0.001950
6	0.009216	-0.065341	1.408534
6	1.223571	-0.007795	2.119132

6	2.438986	0.134176	1.461080
1	3.376474	0.179183	2.023126
6	2.438703	0.176224	0.072228
6	1.238005	0.078698	-0.646966
6	-0.429745	-0.546272	3.732593
1	-0.920179	-0.122898	4.621245
1	-0.519936	-1.640800	3.795646
6	1.062728	-0.174373	3.620497
6	1.415265	1.102712	4.395685
1	1.353094	0.914319	5.478567
1	2.442179	1.425872	4.165059
1	0.731680	1.927329	4.160772
6	1.945784	-1.318559	4.135040
1	1.720017	-1.528508	5.192057
1	1.776101	-2.236588	3.553533
1	3.013268	-1.059755	4.064221
6	3.089651	-0.043067	-2.203036
1	3.298710	-1.098204	-2.430667
1	3.533783	0.560171	-3.007858
6	3.667540	0.289444	-0.810236
6	4.269829	1.700221	-0.748542
1	5.174016	1.754567	-1.374319
1	3.564104	2.458335	-1.111057
1	4.551031	1.956802	0.284281

6	4.742001	-0.727254	-0.408753
1	5.569224	-0.715810	-1.135156
1	5.162491	-0.492732	0.580987
1	4.325407	-1.744707	-0.372599
6	-1.143262	-0.089452	2.416605
6	-1.811926	1.271928	2.602896
6	-1.256884	2.536776	2.627812
1	-0.189435	2.655802	2.428771
6	-2.045603	3.673601	2.896257
6	-3.440000	3.520585	3.053647
6	-3.996574	2.229639	3.002151
1	-5.075655	2.102102	3.111640
6	-3.196107	1.117917	2.785498
6	-3.533874	-0.295580	2.559488
6	-4.751808	-0.957976	2.544853
1	-5.663621	-0.411224	2.794588
6	-4.829940	-2.316077	2.191816
6	-3.646655	-3.005533	1.845799
6	-2.415136	-2.323910	1.892756
1	-1.490557	-2.851489	1.643542
6	-2.356472	-0.984581	2.228147
6	-1.327330	5.024495	3.005547
6	-0.142394	4.915741	3.978852
1	0.285946	5.915081	4.153114

1	-0.464879	4.503987	4.947010
1	0.660553	4.277122	3.583636
6	-0.786042	5.436128	1.628477
1	-1.589198	5.588219	0.892677
1	-0.206588	6.369646	1.708495
1	-0.121287	4.657055	1.228073
6	-2.279919	6.102765	3.543196
1	-2.369903	5.994313	4.636373
1	-1.829058	7.092316	3.366930
6	-4.381421	4.711065	3.267981
6	-4.844368	4.733544	4.734374
1	-5.375440	3.802843	4.982941
1	-3.997348	4.823451	5.428724
1	-5.530382	5.577542	4.907960
6	-5.620328	4.608314	2.364835
1	-5.333637	4.486417	1.309214
1	-6.273217	3.769147	2.641955
1	-6.216228	5.529899	2.454137
6	-3.656590	6.017095	2.911327
1	-3.559979	6.076680	1.813225
1	-4.283903	6.869391	3.217769
6	-3.635132	-4.486316	1.453405
6	1.533236	0.137744	-2.148459
6	1.098963	1.422182	-2.850500

6	1.236132	2.738306	-2.451909
1	1.581314	2.956605	-1.439472
6	0.931450	3.797896	-3.326626
6	0.439660	3.505260	-4.617538
6	0.222141	2.165183	-4.979702
1	-0.190674	1.927446	-5.961624
6	0.539159	1.134238	-4.105888
6	0.381216	-0.323154	-4.215627
6	-0.213925	-1.118768	-5.182869
1	-0.633829	-0.653543	-6.076859
6	-0.297332	-2.512551	-5.018841
6	0.273436	-3.107152	-3.871517
6	0.860767	-2.283111	-2.893070
1	1.278526	-2.726895	-1.985106
6	0.900796	-0.910905	-3.051957
6	1.101409	5.224174	-2.791716
6	2.458139	5.397124	-2.092498
1	2.603855	6.456606	-1.830566
1	2.522941	4.818806	-1.159775
1	3.285039	5.086976	-2.749356
6	-0.019709	5.477689	-1.772080
1	-1.008460	5.447534	-2.249283
1	-0.017438	4.702750	-0.993241
1	0.109870	6.459650	-1.287566

6	1.016730	6.261765	-3.922235
1	0.839304	7.252418	-3.472331
1	1.990880	6.329443	-4.432802
6	0.186651	4.603510	-5.653756
6	-1.029875	4.291672	-6.536170
1	-0.832101	3.474027	-7.243324
1	-1.900858	4.010771	-5.927571
1	-1.292985	5.179758	-7.131347
6	1.423837	4.706501	-6.564219
1	1.581549	3.756570	-7.096048
1	1.286167	5.503844	-7.312091
1	2.337723	4.916602	-5.992011
6	-0.067750	5.936503	-4.934792
1	-0.148795	6.740027	-5.685566
1	-1.043355	5.874468	-4.423574
6	-0.984882	-3.326343	-6.121182
6	-2.316638	-2.679786	-6.531510
1	-2.957385	-2.512490	-5.653152
1	-2.175820	-1.717104	-7.042061
1	-2.849758	-3.345895	-7.227381
6	-0.062646	-3.381161	-7.351195
1	0.160366	-2.366484	-7.712474
1	0.896096	-3.865737	-7.118734
1	-0.546944	-3.938566	-8.168296

6	-1.292252	-4.747117	-5.625057
1	-2.164049	-4.708245	-4.951174
1	-1.593436	-5.365069	-6.486069
6	0.251674	-4.617460	-3.616407
6	-0.773410	-4.912288	-2.509885
1	-1.788612	-4.610472	-2.804576
1	-0.784236	-5.986718	-2.266119
1	-0.520080	-4.354806	-1.596587
6	1.629432	-5.117590	-3.156217
1	1.619877	-6.216838	-3.095335
1	2.413247	-4.818579	-3.867804
1	1.902727	-4.736113	-2.162663
6	-0.116160	-5.375432	-4.899963
1	0.761519	-5.397068	-5.567016
1	-0.334256	-6.423987	-4.641216
6	-3.098873	-5.310127	2.637164
1	-3.731016	-5.200108	3.529468
1	-3.052205	-6.377777	2.370506
1	-2.085501	-4.978920	2.908240
6	-2.726911	-4.722420	0.239456
1	-2.980759	-4.034966	-0.581378
1	-1.664220	-4.586348	0.483081
1	-2.848260	-5.755063	-0.123919
6	-5.049186	-4.952389	1.078415

1	-5.298644	-4.562194	0.077815
1	-5.048198	-6.050823	0.991632
6	-6.217328	-2.966901	2.145709
6	-7.037003	-2.619225	3.397129
1	-7.304947	-1.554547	3.441245
1	-7.976140	-3.193783	3.392551
1	-6.482396	-2.872731	4.312614
6	-6.963463	-2.443592	0.905670
1	-6.427987	-2.688328	-0.022494
1	-7.973713	-2.879111	0.853405
1	-7.062664	-1.348912	0.947851
6	-6.093960	-4.496373	2.080539
1	-5.836365	-4.877287	3.082581
6	-3.292047	0.892993	-0.325592
1	-4.122438	0.899045	0.377885
6	-2.732867	1.678248	-1.208362
6	-2.916563	3.041150	-1.699145
6	-3.260767	4.051232	-0.784685
1	-3.266491	3.814510	0.283371
6	-3.585355	5.325756	-1.231335
1	-3.838419	6.092783	-0.494634
6	-3.600225	5.642854	-2.599574
6	-3.248428	4.629489	-3.497566
1	-3.253270	4.831886	-4.567349

6	-2.882675	3.355384	-3.059472
1	-2.592635	2.583920	-3.777202
6	-3.938779	7.067056	-3.048511
6	-5.295260	7.488523	-2.461452
1	-6.093033	6.811424	-2.800695
1	-5.546653	8.510264	-2.784590
1	-5.285777	7.477921	-1.362414
6	-2.840298	8.016861	-2.540395
1	-2.750687	7.977118	-1.444544
1	-3.067802	9.054818	-2.829029
1	-1.862681	7.745284	-2.967935
6	-4.015680	7.184953	-4.573878
1	-3.050683	6.952953	-5.049018
1	-4.283991	8.214925	-4.850836
1	-4.778454	6.511146	-4.991612
51	-1.794424	-0.292726	-1.303077
1	-7.080467	-4.920163	1.833111

Table S31

[Bi-Prod]¹

E : -3473.76122541 Hartree

G : -3472.218462 Hartree

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	-0.007508	-0.031295	-0.008278
6	-0.013948	-0.050039	1.401237
6	1.186202	0.003756	2.137131
6	2.418130	0.114284	1.503396
1	3.343971	0.155864	2.084746
6	2.447175	0.130413	0.114147
6	1.258678	0.038688	-0.626157
6	-0.509792	-0.480092	3.725019
1	-1.012498	-0.028209	4.592569
1	-0.616675	-1.571238	3.813899
6	0.990472	-0.132229	3.637300
6	1.346455	1.153694	4.395843
1	1.256084	0.988295	5.480555
1	2.383541	1.455617	4.182714
1	0.682280	1.984248	4.128673
6	1.844547	-1.279547	4.192333
1	1.593581	-1.465729	5.248172
1	1.672704	-2.205893	3.624763
1	2.917189	-1.038476	4.139007
6	3.136429	-0.133784	-2.145838
1	3.330474	-1.196396	-2.351745

1	3.606820	0.447763	-2.951806
6	3.693575	0.212017	-0.747386
6	4.314718	1.615159	-0.697997
1	5.231267	1.646534	-1.307235
1	3.626637	2.376865	-1.086331
1	4.579867	1.885070	0.335640
6	4.746185	-0.812839	-0.310703
1	5.586951	-0.824587	-1.021480
1	5.151223	-0.568278	0.683031
1	4.314527	-1.823655	-0.265940
6	-1.189496	-0.046553	2.382292
6	-1.861556	1.318094	2.532507
6	-1.306085	2.582648	2.576822
1	-0.234324	2.701723	2.402932
6	-2.098358	3.718110	2.842515
6	-3.495776	3.566086	2.972593
6	-4.053361	2.277344	2.892364
1	-5.134188	2.149801	2.982799
6	-3.249840	1.166514	2.683852
6	-3.583009	-0.249721	2.472337
6	-4.800159	-0.913855	2.453589
1	-5.716470	-0.361979	2.674192
6	-4.870817	-2.280493	2.135242
6	-3.680270	-2.977114	1.829823

6	-2.450842	-2.292639	1.880878
1	-1.520792	-2.825261	1.664985
6	-2.398910	-0.944657	2.181820
6	-1.381464	5.067280	2.980962
6	-0.207979	4.946701	3.966540
1	0.216600	5.944227	4.159536
1	-0.541037	4.521158	4.925109
1	0.600821	4.315100	3.572162
6	-0.823983	5.497792	1.616319
1	-1.617339	5.643173	0.868549
1	-0.258876	6.438594	1.712875
1	-0.141989	4.731297	1.221530
6	-2.340202	6.138158	3.522606
1	-2.444538	6.013043	4.612706
1	-1.885687	7.129644	3.367762
6	-4.438665	4.753801	3.196691
6	-4.916195	4.750136	4.658756
1	-5.452693	3.816618	4.883959
1	-4.075880	4.823513	5.363089
1	-5.601144	5.593087	4.841632
6	-5.669337	4.669560	2.280670
1	-5.374162	4.568846	1.225296
1	-6.324926	3.825412	2.535401
1	-6.265703	5.589448	2.383409

6	-3.708667	6.065033	2.871851
1	-3.598174	6.143407	1.776358
1	-4.339004	6.912666	3.185051
6	-3.660288	-4.469044	1.482031
6	1.583417	0.075629	-2.122407
6	1.178793	1.361160	-2.838610
6	1.308131	2.675588	-2.433428
1	1.641431	2.889672	-1.416239
6	0.998087	3.737521	-3.302917
6	0.511816	3.449893	-4.597054
6	0.310850	2.110067	-4.969824
1	-0.098135	1.875377	-5.954105
6	0.631821	1.076922	-4.100336
6	0.462344	-0.379307	-4.209023
6	-0.127609	-1.171396	-5.182108
1	-0.518511	-0.705470	-6.088733
6	-0.242997	-2.562528	-5.009016
6	0.286115	-3.158451	-3.842914
6	0.868842	-2.337385	-2.857430
1	1.257831	-2.781238	-1.936820
6	0.947253	-0.967911	-3.029246
6	1.145018	5.161015	-2.755896
6	2.487381	5.344123	-2.032203
1	2.616566	6.403452	-1.761268

1	2.542738	4.760817	-1.102052
1	3.328950	5.047553	-2.676551
6	0.003266	5.393557	-1.754199
1	-0.977336	5.354726	-2.247539
1	0.002174	4.611946	-0.981920
1	0.112100	6.372947	-1.259378
6	1.069437	6.202706	-3.882477
1	0.891437	7.192377	-3.430383
1	2.047201	6.269112	-4.386633
6	0.243220	4.552105	-5.625608
6	-0.983593	4.238040	-6.493069
1	-0.793527	3.421786	-7.203981
1	-1.845092	3.955385	-5.871729
1	-1.256689	5.126445	-7.083427
6	1.469289	4.664795	-6.549469
1	1.631489	3.715518	-7.081182
1	1.315604	5.459110	-7.297360
1	2.386676	4.886045	-5.986992
6	-0.010325	5.882606	-4.901582
1	-0.086799	6.688838	-5.650008
1	-0.988355	5.821298	-4.395368
6	-0.917440	-3.372002	-6.122573
6	-2.223226	-2.702111	-6.576516
1	-2.886074	-2.513925	-5.718903

1	-2.048441	-1.747402	-7.091446
1	-2.749954	-3.363748	-7.281344
6	0.037641	-3.457351	-7.325561
1	0.292220	-2.450975	-7.689113
1	0.978949	-3.959860	-7.061959
1	-0.435310	-4.011987	-8.151087
6	-1.267852	-4.781328	-5.622467
1	-2.156071	-4.718457	-4.972120
1	-1.559596	-5.400600	-6.485715
6	0.227897	-4.665852	-3.576279
6	-0.828839	-4.931106	-2.492511
1	-1.830726	-4.612309	-2.814350
1	-0.867980	-6.002951	-2.240833
1	-0.585486	-4.373012	-1.576884
6	1.584016	-5.189123	-3.078809
1	1.551408	-6.287461	-3.010857
1	2.390705	-4.910586	-3.772881
1	1.840393	-4.806029	-2.081402
6	-0.124107	-5.427432	-4.862160
1	0.769203	-5.473543	-5.506700
1	-0.370648	-6.468733	-4.599933
6	-3.142019	-5.256285	2.698221
1	-3.788814	-5.120291	3.576320
1	-3.089806	-6.331474	2.464846

1	-2.133709	-4.915101	2.975663
6	-2.732694	-4.739536	0.290457
1	-2.980507	-4.081301	-0.555751
1	-1.674498	-4.587697	0.544407
1	-2.842494	-5.784214	-0.040859
6	-5.067012	-4.949660	1.097723
1	-5.300520	-4.590719	0.081617
1	-5.062749	-6.050258	1.044633
6	-6.256291	-2.934890	2.082934
6	-7.100500	-2.550899	3.307135
1	-7.371396	-1.486106	3.313160
1	-8.038241	-3.127751	3.302420
1	-6.562952	-2.774479	4.240405
6	-6.979429	-2.451013	0.813626
1	-6.425719	-2.722249	-0.096305
1	-7.987892	-2.889915	0.754925
1	-7.081014	-1.355693	0.821091
6	-6.129519	-4.465347	2.067312
1	-5.888273	-4.814386	3.084916
6	-3.461416	0.866225	-0.445288
1	-4.299344	0.793222	0.244771
6	-2.897201	1.698151	-1.264892
6	-3.023596	3.072373	-1.734914
6	-3.310247	4.091237	-0.810725

1	-3.327107	3.845967	0.254773
6	-3.565146	5.385609	-1.246555
1	-3.776246	6.158334	-0.502673
6	-3.561078	5.717665	-2.610919
6	-3.265846	4.695126	-3.519265
1	-3.255679	4.907231	-4.587441
6	-2.972551	3.399230	-3.092596
1	-2.722450	2.620095	-3.817095
6	-3.816149	7.163803	-3.044557
6	-5.147998	7.656063	-2.456360
1	-5.982344	7.030314	-2.806100
1	-5.338710	8.694441	-2.767798
1	-5.143025	7.631781	-1.357500
6	-2.666234	8.042813	-2.523048
1	-2.584355	7.988109	-1.427172
1	-2.830608	9.094934	-2.803213
1	-1.704372	7.717120	-2.948636
6	-3.880771	7.302596	-4.568668
1	-2.928973	7.020047	-5.043034
1	-4.087962	8.349329	-4.835052
1	-4.679799	6.678660	-4.996031
83	-1.810876	-0.322922	-1.449194
1	-7.110870	-4.898947	1.816337

