Supporting Information

The Theoretical Investigations of the Reactivity of Neutral Molecules that Feature an M=M (M = B, Al, Ga, In, and Tl) Double Bond

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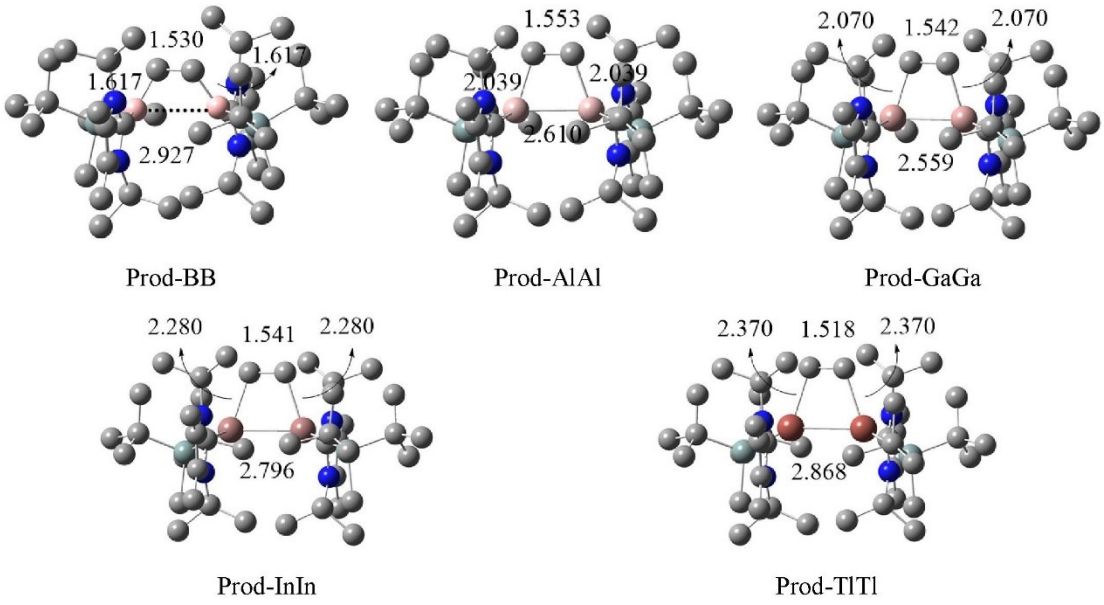

Figure S1. The optimized Prod structures at the level of B3LYP-D3(BJ)/def2-SVP. The hydrogen atoms are omitted for clarity.

Table S1. The calculated energy difference (eV) for $\pi_{EE} \rightarrow \pi_{EE}^*$ ($\Delta E(\pi_E \rightarrow \pi_{EE}^*)$) and HOMO-LUMO gap ($\Delta E$(H-L)) at B3LYP-D3(BJ)/def2-SVP level of theory

	$\Delta E(\pi_{EE} \rightarrow \pi_{EE}^*)$	ΔE(H-L)
BB	3.77	3.17
AlAl	2.56	2.20
GaGa	2.55	2.55
InIn	2.26	2.26
TlTl	2.31	2.30

Table S2. BP86-D3(BJ) ETS[(a)] energy decomposition results (in kcal mol^{-1}) describing the bond between ethene and **Rea-BB**. Singlet and triplet spin states were considered in ETS-NOCV analysis.

ETS results	Rea	TS	Prod	$\Delta E^{\#}$[ΔE(TS)-ΔE(Rea)]	ΔE_{rxn}[ΔE(Prod)-ΔE(Rea)]
Fragments in the singlet spin state					
ΔE[(b)]	0.0	47.6	-20.1	47.6	-20.1
ΔE_{orb}	0.0	-100.8	-656.4	-100.8	-656.4
ΔE_{Pauli}	0.0	209.0	781.3	209.0	781.3
ΔE_{elstat}	0.0	-106.1	-315.3	-106.1	-315.3
ΔE_{disper}	0.0	-19.3	-16.1	-19.3	-16.1
ΔE_{dist}	0.0	64.8	186.4	64.8	186.4
Fragments in the triplet spin state					
ΔE_{total}[(b)]	0.0	47.6	-20.1	47.6	-20.1
ΔE_{orb}	-92.3	-153.7	-412.7	-61.4	-320.4
ΔE_{Pauli}	0.0	157.0	557.7	157.0	557.7
ΔE_{elstat}	0.0	-98.3	-323.9	-98.3	-323.9
ΔE_{disper}	0.0	-19.3	-16.1	-19.3	-16.1
ΔE_{dist}	92.3	161.9	174.9	69.6	82.6

[(a)] $\Delta E = \Delta E_{orb} + \Delta E_{Pauli} + \Delta E_{elstat} + \Delta E_{disper} + \Delta E_{dist}$

[(b)] Fragments in singlet state were considered in ETS analysis.

[(c)] Fragments in triplet state were considered in ETS analysis. Distortion energy, ΔE_{dist}, calculated with respect to the singlet ground state of ethene and **Rea-BB**.

Table S3. BP86-D3(BJ) ETS[(a)] energy decomposition results (in kcal mol^{-1}) describing the bond between ethene and **Rea-GaGa**. Singlet and triplet spin states were considered in ETS-NOCV analysis.

ETS results	Rea	TS	Prod	$\Delta E^{\#}$[ΔE(TS)-ΔE(Rea)]	ΔE_{rxn}[ΔE(Prod)-ΔE(Rea)]
Fragments in the singlet spin state					
ΔE[(b)]	0.0	9.2	-40.3	9.2	-40.3
ΔE_{orb}	0.0	-30.3	-344.8	-30.3	-344.8
ΔE_{Pauli}	0.0	68.0	477.0	68.0	477.0
ΔE_{elstat}	0.0	-34.4	-236.7	-34.4	-236.7
ΔE_{disper}	0.0	-13.9	-16.6	-13.9	-16.6
ΔE_{dist}	0.0	19.8	80.8	19.8	80.8
Fragments in the triplet spin state					
ΔE[(c)]	0.0	9.2	-40.3	9.2	-40.3
ΔE_{orb}	-81.5	-137.6	-233.8	-56.1	-152.3
ΔE_{Pauli}	0.0	75.2	325.9	75.2	325.9
ΔE_{elstat}	0.0	-50.1	-221.7	-50.1	-221.7
ΔE_{disper}	0.0	-13.9	-16.6	-13.9	-16.6
ΔE_{dist}	81.5	135.6	105.9	54.1	24.4

[(a)] $\Delta E = \Delta E_{orb} + \Delta E_{Pauli} + \Delta E_{elstat} + \Delta E_{disper} + \Delta E_{dist}$

[(b)] Fragments in singlet state were considered in ETS analysis.

[(c)] Fragments in triplet state were considered in ETS analysis. Distortion energy, ΔE_{dist}, calculated with respect to the singlet ground state of ethene and **Rea-GaGa**.

Table S4. BP86-D3(BJ) ETS[(a)] energy decomposition results (in kcal mol^{-1}) describing the bond between ethene and **Rea-InIn**. Singlet and triplet spin states were considered in ETS-NOCV analysis.

ETS results	Rea	TS	Prod	$\Delta E^{\#}$[ΔE(TS)-ΔE(Rea)]	ΔE_{rxn}[ΔE(Prod)-ΔE(Rea)]
Fragments in the singlet spin state					
ΔE[(b)]	0.0	1.2	-28.1	1.2	-28.1
ΔE_{orb}	0.0	-46.0	-276.0	-46.0	-276.0
ΔE_{Pauli}	0.0	95.4	391.8	95.4	391.8
ΔE_{elstat}	0.0	-51.2	-203.9	-51.2	-203.9
ΔE_{disper}	0.0	-13.8	-15.0	-13.8	-15.0
ΔE_{dist}	0.0	16.8	75.0	16.8	75.0
Fragments in the triplet spin state					
ΔE[(c)]	0.0	1.2	-28.1	1.2	-28.1
ΔE_{orb}	-79.8	-132.8	-193.8	-53.0	-114.0
ΔE_{Pauli}	0.0	91.6	269.5	91.6	269.5
ΔE_{elstat}	0.0	-65.5	-191.1	-65.5	-191.1
ΔE_{disper}	0.0	-13.8	-15.0	-13.8	-15.0
ΔE_{dist}	79.8	121.7	102.3	41.9	22.5

[(a)] $\Delta E = \Delta E_{orb} + \Delta E_{Pauli} + \Delta E_{elstat} + \Delta E_{disper} + \Delta E_{dist}$

[(b)] Fragments in singlet state were considered in ETS analysis.

[(c)] Fragments in triplet state were considered in ETS analysis. Distortion energy, ΔE_{dist}, calculated with respect to the singlet ground state of ethene and **Rea-InIn**.

Table S5. BP86-D3(BJ) ETS[(a)] energy decomposition results (in kcal mol^{-1}) describing the bond between ethene and **Rea-TlTl**. Singlet and triplet spin states were considered in ETS-NOCV analysis.

ETS results	Rea	TS	Prod	$\Delta E^{\#}$[ΔE(TS)-ΔE(Rea)]	ΔE_{rxn}[ΔE(Prod)-ΔE(Rea)]
Fragments in the singlet spin state					
ΔE[(b)]	0.0	5.2	-4.6	5.2	-4.6
ΔE_{orb}	0.0	-75.0	-226.8	-75.0	-226.8
ΔE_{Pauli}	0.0	136.5	339.4	136.5	339.4
ΔE_{elstat}	0.0	-77.2	-181.5	-77.2	-181.5
ΔE_{disper}	0.0	-12.7	-14.2	-12.7	-14.2
ΔE_{dist}	0.0	25.6	78.5	25.6	78.5
Fragments in the triplet spin state					
ΔE[(b)]	0.0	5.2	-4.6	5.2	-4.6
ΔE_{orb}	-87.1	-134.3	-168.2	-47.2	-81.1
ΔE_{Pauli}	0.0	122.1	237.6	122.1	237.6
ΔE_{elstat}	0.0	-88.7	-168.7	-88.7	-168.7
ΔE_{disper}	0.0	-12.7	-14.2	-12.7	-14.2
ΔE_{dist}	87.1	118.8	108.9	31.7	21.8

[(a)] $\Delta E = \Delta E_{orb} + \Delta E_{Pauli} + \Delta E_{elstat} + \Delta E_{disper} + \Delta E_{dist}$

[(b)] Fragments in singlet state were considered in ETS analysis.

[(c)] Fragments in triplet state were considered in ETS analysis. Distortion energy, ΔE_{dist}, calculated with respect to the singlet ground state of ethene and **Rea-TlTl**.

Table S2

B3LYP-D3(BJ)/def2-SVP

Rea-BB

Atomic Number	Coordinates (Angstroms) X	Y	Z
5	-0.741657	-0.342984	-0.006124
5	0.741639	0.343020	-0.006097
7	-2.459303	0.907208	1.546038
7	-2.997579	1.090380	-0.543665
6	-2.055746	0.528937	0.284599
6	-3.587154	1.725132	1.495382
6	-3.925950	1.844359	0.177762
6	-1.804661	0.440358	2.778372
1	-1.092480	-0.301053	2.391743
6	-0.998787	1.534951	3.469321
1	-1.626991	2.363452	3.826603
1	-0.246314	1.944673	2.789874
1	-0.483884	1.113176	4.345786
6	-2.780953	-0.250652	3.734597
1	-3.476297	-0.907217	3.194821
1	-3.363542	0.464141	4.332305
1	-2.211246	-0.874670	4.439283
6	-3.076925	0.825514	-1.987806
1	-2.190209	0.205471	-2.171952
6	-2.978210	2.086262	-2.850830
1	-2.718127	1.797461	-3.879682
1	-2.197950	2.766157	-2.491751
1	-3.929446	2.634127	-2.893732
6	-4.331812	0.019701	-2.333650
1	-4.454507	-0.833263	-1.656383
1	-4.255478	-0.359199	-3.362741
1	-5.240427	0.634977	-2.278695
6	-4.261166	2.347131	2.673823
1	-4.854720	1.620739	3.250541
1	-4.946686	3.134589	2.335239
1	-3.545782	2.813701	3.364424

6	-5.000348	2.696227	-0.413644
1	-5.672782	2.141022	-1.081882
1	-4.582966	3.538935	-0.986660
1	-5.618172	3.118316	0.388942
14	-0.951735	-2.360901	-0.348815
6	0.618963	-3.327703	0.177163
1	0.439313	-4.412863	0.143641
1	0.934518	-3.073712	1.195658
1	1.468020	-3.117460	-0.483957
6	-1.130109	-2.868778	-2.275777
6	-2.576211	-3.002286	-2.775853
1	-2.584891	-3.159335	-3.871481
1	-3.166149	-2.103798	-2.576754
1	-3.106865	-3.853542	-2.328975
6	-0.431904	-4.215788	-2.550629
1	-0.847547	-5.032462	-1.942996
1	0.649096	-4.181998	-2.355962
1	-1.074517	-0.888983	-3.222697
6	-1.974372	-3.294038	2.147677
1	-1.781466	-2.281420	2.515862
1	-1.069585	-3.893749	2.328144
6	-3.721765	-2.578002	0.519540
1	-4.101702	-2.624099	-0.511188
1	-3.652349	-1.516620	0.801613
1	-4.487990	-3.044154	1.168468
6	-2.545406	-4.774693	0.264967
1	-3.286721	-5.262645	0.926559
1	-1.604877	-5.338058	0.367305
1	-2.900229	-4.904838	-0.765426
1	-0.561127	-4.497377	-3.612846
6	-0.452322	-1.789489	-3.136454
1	-0.271104	-2.161128	-4.162750
1	0.498150	-1.453001	-2.712730
6	-2.371461	-3.298376	0.662862
1	-2.782461	-3.723456	2.769953
7	2.997625	-1.090291	-0.543609
7	2.459270	-0.907167	1.546079
6	2.055738	-0.528896	0.284633

6	3.926012	-1.844231	0.177838
6	3.587159	-1.725042	1.495449
6	3.076826	-0.825599	-1.987786
1	2.190085	-0.205641	-2.171945
6	2.978060	-2.086437	-2.850655
1	3.929286	-2.634328	-2.893492
1	2.197796	-2.766303	-2.491496
1	2.717983	-1.797738	-3.879537
6	4.331656	-0.019805	-2.333876
1	4.454558	0.833079	-1.656550
1	5.240248	-0.635139	-2.279249
1	4.255055	0.359205	-3.362906
6	1.804555	-0.440396	2.778410
1	1.092369	0.301018	2.391799
6	0.998672	-1.535059	3.469236
1	0.483739	-1.113381	4.345730
1	0.246227	-1.944707	2.789720
1	1.626871	-2.363595	3.826447
6	2.780773	0.250585	3.734724
1	3.476104	0.907226	3.195021
1	2.211005	0.874531	4.439425
1	3.363364	-0.464220	4.332414
6	5.000500	-2.696009	-0.413538
1	5.672500	-2.140843	-1.082247
1	5.618751	-3.117500	0.389032
1	4.583232	-3.539139	-0.986020
6	4.261174	-2.346993	2.673918
1	4.854724	-1.620575	3.250607
1	3.545787	-2.813529	3.364537
1	4.946684	-3.134476	2.335375
6	1.130249	2.868827	-2.275779
6	0.432116	4.215859	-2.550688
1	0.561460	4.497462	-3.612887
1	-0.648906	4.182093	-2.356140
1	0.847718	5.032513	-1.942997
6	2.576426	3.002292	-2.775636
1	3.107113	3.853411	-2.328540
1	3.166224	2.103708	-2.576635

1	-0.498281	1.453379	-2.713594
6	2.545430	4.774618	0.265098
1	2.900308	4.904777	-0.765273
1	1.604909	5.338003	0.367396
14	0.951689	2.360902	-0.348814
6	-0.618943	3.327791	0.177162
1	-0.439215	4.412941	0.143693
1	-1.467989	3.117639	-0.483968
1	-0.934550	3.073779	1.195641
1	2.585268	3.159530	-3.871235
6	0.452586	1.789587	-3.136644
1	0.272088	2.161140	-4.163098
1	1.074467	0.888849	-3.222348
6	2.371424	3.298297	0.662942
6	1.974255	3.293925	2.147735
1	1.069519	3.893720	2.328181
1	1.781219	2.281307	2.515850
1	2.782351	3.723226	2.770082
6	3.721709	2.577867	0.519653
1	4.487925	3.043942	1.168647
1	3.652239	1.516467	0.801655
1	4.101694	2.624007	-0.511056
1	3.286722	5.262536	0.926742

Table S3

B3LYP-D3(BJ)/def2-SVP

Rea-AlAl

Atomic Number	Coordinates (Angstroms) X	Y	Z
13	-1.173594	-0.198060	0.007336
13	1.173745	0.197867	0.008439
7	-2.389997	2.349405	1.215591
7	-2.592327	2.373836	-0.936502
6	-2.198082	1.589410	0.101902
6	-2.867250	3.615156	0.878319
6	-2.992524	3.632011	-0.489247
6	-2.087096	1.839936	2.569128
1	-1.867355	0.772445	2.384796
6	-0.807397	2.450162	3.127226
1	-0.869375	3.542874	3.239453
1	0.034925	2.202656	2.466628
1	-0.596141	2.018876	4.118012
6	-3.282709	1.928453	3.516251
1	-4.203502	1.576263	3.029684
1	-3.452147	2.945336	3.898196
1	-3.094559	1.279518	4.385109
6	-2.504908	1.903837	-2.333109
1	-2.313123	0.824794	-2.220814
6	-1.287397	2.493230	-3.036340
1	-1.212952	2.086621	-4.056675
1	-0.378269	2.203480	-2.490469
1	-1.333125	3.590566	-3.109568
6	-3.816165	2.066702	-3.098950
1	-4.671869	1.729122	-2.495629
1	-3.778053	1.442641	-4.004477
1	-3.998993	3.101776	-3.419638
6	-3.190038	4.700177	1.850689
1	-4.116913	4.495551	2.410009
1	-3.331433	5.649336	1.316724
1	-2.385993	4.849654	2.585008

6	-3.470678	4.743945	-1.362815
1	-4.490366	4.569537	-1.742063
1	-2.814535	4.895006	-2.231542
1	-3.487326	5.683164	-0.793962
14	-2.549569	-2.232127	-0.105950
6	-1.362653	-3.729649	0.039060
1	-1.903516	-4.678443	0.191967
1	-0.656531	-3.602212	0.872395
1	-0.763042	-3.827030	-0.880257
6	-3.482157	-2.504127	-1.817636
6	-4.672030	-1.539570	-1.941114
1	-5.097943	-1.569339	-2.961875
1	-4.378266	-0.498214	-1.734018
1	-5.482732	-1.797759	-1.243378
6	-3.980149	-3.949013	-2.000751
1	-4.724546	-4.238872	-1.247467
1	-3.152970	-4.674151	-1.947590
1	-2.041887	-1.211817	-2.877539
6	-2.938748	-2.471064	2.690100
1	-2.216761	-1.642944	2.777284
1	-2.367984	-3.412612	2.711090
6	-4.618790	-1.051187	1.523564
1	-5.306319	-0.924141	0.675385
1	-3.972634	-0.162053	1.553928
1	-5.229817	-1.055555	2.446311
6	-4.746952	-3.543922	1.352464
1	-5.327982	-3.623065	2.291045
1	-4.209667	-4.496981	1.220435
1	-5.474355	-3.451121	0.532260
1	-4.454660	-4.067901	-2.993583
6	-2.493271	-2.212966	-2.959883
1	-3.002723	-2.286735	-3.939424
1	-1.663857	-2.936627	-2.969760
6	-3.790674	-2.342658	1.414693
1	-3.583906	-2.454507	3.588723
7	2.592242	-2.373616	-0.936924
7	2.390968	-2.349718	1.215272
6	2.198484	-1.589471	0.101863

6	2.992705	-3.631888	-0.490173
6	2.868114	-3.615368	0.877464
6	2.503961	-1.903281	-2.333371
1	2.312468	-0.824230	-2.220678
6	1.285819	-2.492257	-3.035849
1	1.331093	-3.589619	-3.109019
1	0.377138	-2.202071	-2.489445
1	1.210910	-2.085681	-4.056164
6	3.814633	-2.066203	-3.100194
1	4.670846	-1.728934	-2.497418
1	3.997033	-3.101222	-3.421300
1	3.775967	-1.441891	-4.005524
6	2.088255	-1.840708	2.569021
1	1.868350	-0.773177	2.385082
6	0.808684	-2.451276	3.127064
1	0.597494	-2.020393	4.118039
1	-0.033737	-2.203616	2.466640
1	0.870800	-3.544024	3.238855
6	3.284033	-1.929352	3.515912
1	4.204651	-1.576710	3.029332
1	3.095868	-1.280851	4.385090
1	3.453804	-2.946361	3.897371
6	3.470398	-4.743593	-1.364281
1	4.489772	-4.568953	-1.744262
1	3.487612	-5.682911	-0.795611
1	2.813627	-4.894589	-2.232550
6	3.191477	-4.700575	1.849437
1	4.118564	-4.495933	2.408403
1	2.387777	-4.850352	2.584076
1	3.332787	-5.649586	1.315188
6	3.481403	2.503905	-1.818131
6	3.979084	3.948845	-2.001664
1	4.453351	4.067614	-2.994627
1	3.151772	4.673829	-1.948474
1	4.723582	4.239011	-1.248602
6	4.671401	1.539520	-1.941736
1	5.482234	1.797974	-1.244252
1	4.377860	0.498151	-1.734378

1	1.662734	2.935909	-2.969829
6	4.747103	3.544493	1.351266
1	5.474351	3.451453	0.530950
1	4.209733	4.497473	1.219013
14	2.549345	2.232109	-0.106112
6	1.362215	3.729462	0.038924
1	1.902948	4.678344	0.191745
1	0.762517	3.826703	-0.880350
1	0.656173	3.601946	0.872314
1	5.097052	1.569174	-2.962610
6	2.492250	2.212365	-2.960043
1	3.001415	2.286017	-3.939742
1	2.041022	1.211180	-2.877375
6	3.790918	2.343180	1.414124
6	2.939412	2.471888	2.689776
1	2.368428	3.413306	2.710615
1	2.217670	1.643618	2.777531
1	3.584895	2.455823	3.588174
6	4.619182	1.051811	1.523142
1	5.230680	1.056638	2.445576
1	3.973114	0.162637	1.554261
1	5.306282	0.924423	0.674667
1	5.328320	3.623998	2.289700

Table S4

B3LYP-D3(BJ)/def2-SVP

Rea-GaGa

Atomic Number	Coordinates (Angstroms) X	Y	Z
31	-1.107974	-0.228451	-0.257166
31	1.125132	0.257875	0.248809
7	-2.336392	2.210619	1.290161
7	-2.750164	2.304124	-0.829530
6	-2.224722	1.501692	0.133764
6	-2.895469	3.467992	1.049277
6	-3.156188	3.527465	-0.296504
6	-1.943868	1.647955	2.598479
1	-1.712470	0.599892	2.351816
6	-0.654313	2.260725	3.128493
1	-0.727042	3.347714	3.281593
1	0.166260	2.043929	2.431695
1	-0.401807	1.798812	4.095698
6	-3.088146	1.669308	3.613135
1	-4.036185	1.353402	3.156314
1	-3.229815	2.658149	4.072049
1	-2.856031	0.961864	4.423610
6	-2.768363	1.888496	-2.244084
1	-2.508673	0.819261	-2.190274
6	-1.652222	2.570303	-3.028017
1	-1.634421	2.192404	-4.061812
1	-0.686008	2.331081	-2.562091
1	-1.773875	3.663477	-3.067038
6	-4.150646	2.004872	-2.882424
1	-4.927953	1.600673	-2.217195
1	-4.165075	1.416076	-3.812010
1	-4.414958	3.039298	-3.143577
6	-3.157020	4.506977	2.088020
1	-4.026582	4.260616	2.718054
1	-3.363850	5.471655	1.605469
1	-2.294311	4.648028	2.753852

6	-3.770878	4.643321	-1.074083
1	-4.811943	4.426751	-1.362976
1	-3.210768	4.865885	-1.993608
1	-3.782925	5.557732	-0.465895
14	-2.409952	-2.283131	-0.072862
6	-1.143100	-3.717919	-0.006530
1	-1.607549	-4.676970	0.276993
1	-0.340836	-3.500964	0.714677
1	-0.663639	-3.855446	-0.988048
6	-3.486913	-2.615145	-1.683159
6	-4.707717	-1.682041	-1.721679
1	-5.214280	-1.741500	-2.703308
1	-4.420397	-0.631033	-1.558993
1	-5.453101	-1.944554	-0.956522
6	-3.958419	-4.076897	-1.787704
1	-4.636014	-4.363128	-0.972345
1	-3.110561	-4.779900	-1.778539
1	-2.228928	-1.296810	-2.924954
6	-2.504524	-2.442604	2.747483
1	-1.834960	-1.568038	2.732607
1	-1.871517	-3.343486	2.740685
6	-4.406559	-1.202890	1.716188
1	-5.213333	-1.195937	0.970190
1	-3.849020	-0.263277	1.600504
1	-4.882431	-1.195733	2.715042
6	-4.339622	-3.701514	1.630056
1	-4.817207	-3.792988	2.624108
1	-3.741402	-4.613066	1.470773
1	-5.147934	-3.694971	0.884619
1	-4.503833	-4.235946	-2.737391
6	-2.624518	-2.324401	-2.924227
1	-3.221995	-2.464051	-3.844883
1	-1.762217	-3.004423	-2.991320
6	-3.486758	-2.425038	1.562929
1	-3.055570	-2.433102	3.706615
7	2.522715	-2.252177	-1.028933
7	2.592111	-2.299559	1.129406
6	2.243872	-1.512880	0.075369

6	3.011833	-3.511590	-0.678344
6	3.057160	-3.541151	0.692859
6	2.297528	-1.725640	-2.387998
1	2.075357	-0.664925	-2.201140
6	1.053248	-2.329635	-3.025295
1	1.130358	-3.420080	-3.152990
1	0.177939	-2.097379	-2.404948
1	0.889439	-1.881421	-4.017380
6	3.543404	-1.803354	-3.269905
1	4.441974	-1.486894	-2.720609
1	3.716099	-2.809750	-3.676777
1	3.415604	-1.120297	-4.123007
6	2.415720	-1.848872	2.524016
1	2.151245	-0.784403	2.406244
6	1.212467	-2.519914	3.177095
1	1.074848	-2.125098	4.195610
1	0.306983	-2.289363	2.600485
1	1.322305	-3.612269	3.249674
6	3.701832	-1.933626	3.343105
1	4.553473	-1.515079	2.787430
1	3.577832	-1.342142	4.263050
1	3.949101	-2.961315	3.644706
6	3.411735	-4.576417	-1.644430
1	4.362325	-4.345301	-2.151132
1	3.544157	-5.529808	-1.115585
1	2.651204	-4.732513	-2.422891
6	3.529240	-4.643900	1.581123
1	4.510925	-4.425145	2.031173
1	2.825871	-4.844609	2.401537
1	3.632820	-5.570189	1.000508
6	3.213371	2.555922	-1.933986
6	3.627767	4.019305	-2.176262
1	4.040369	4.134490	-3.196721
1	2.769202	4.703821	-2.094771
1	4.396278	4.364706	-1.472918
6	4.440825	1.648574	-2.106969
1	5.282117	1.976035	-1.478192
1	4.219170	0.603189	-1.842445

1	1.307421	2.872796	-2.971793
6	4.620606	3.751937	1.105474
1	5.291875	3.668131	0.238429
1	4.027401	4.672711	0.984628
14	2.400519	2.295673	-0.158730
6	1.163268	3.745984	0.014953
1	1.670815	4.718613	0.125473
1	0.517926	3.801534	-0.876299
1	0.501772	3.606249	0.881192
1	4.793916	1.660660	-3.155479
6	2.176242	2.199157	-3.011881
1	2.620617	2.300082	-4.020141
1	1.791539	1.174751	-2.907053
6	3.733626	2.508070	1.270683
6	2.972959	2.638301	2.602405
1	2.332880	3.533949	2.626705
1	2.329272	1.764219	2.786989
1	3.685572	2.717285	3.444941
6	4.631262	1.261726	1.355723
1	5.295105	1.317491	2.239358
1	4.033601	0.342986	1.442639
1	5.272384	1.148956	0.470200
1	5.260369	3.889244	1.997840

Table S5

B3LYP-D3(BJ)/def2-SVP

Rea-InIn

Atomic Number	Coordinates (Angstroms) X	Y	Z
49	-1.286356	-0.585195	0.371472
49	1.190238	0.087921	-0.736058
7	-2.880029	2.254305	1.143952
7	-2.488541	2.390196	-0.971173
6	-2.446011	1.529823	0.078466
6	-3.183746	3.566895	0.773901
6	-2.936047	3.652962	-0.572122
6	-2.952677	1.670997	2.495676
1	-2.706075	0.611288	2.328278
6	-1.870270	2.228441	3.417231
1	-2.005734	3.299130	3.628799
1	-0.878625	2.080892	2.968960
1	-1.892244	1.690862	4.377509
6	-4.361345	1.731079	3.082845
1	-5.104328	1.383496	2.350326
1	-4.637203	2.742795	3.412576
1	-4.417254	1.069668	3.960499
6	-2.114266	1.968418	-2.333946
1	-1.861507	0.907482	-2.202688
6	-0.851556	2.659307	-2.835269
1	-0.538343	2.198457	-3.783838
1	-0.033648	2.522788	-2.118718
1	-0.994817	3.734633	-3.014894
6	-3.283052	2.063612	-3.313697
1	-4.189865	1.609710	-2.891827
1	-3.028157	1.513493	-4.231744
1	-3.506209	3.101551	-3.600518
6	-3.708197	4.623883	1.688481
1	-4.755604	4.442104	1.978573
1	-3.671688	5.600227	1.187499
1	-3.118001	4.706773	2.611931

6	-3.125371	4.828566	-1.472219
1	-3.967963	4.689043	-2.168004
1	-2.230621	5.039814	-2.074417
1	-3.339048	5.724649	-0.874673
14	-2.997265	-2.477266	-0.476688
6	-1.986314	-4.060254	-0.840216
1	-2.630304	-4.933045	-1.041581
1	-1.330604	-4.320640	0.003412
1	-1.339786	-3.904906	-1.718458
6	-3.985928	-2.124930	-2.131354
6	-4.996009	-0.988872	-1.909621
1	-5.432987	-0.656609	-2.870216
1	-4.525692	-0.115946	-1.428987
1	-5.831761	-1.309022	-1.268053
6	-4.720813	-3.363597	-2.672783
1	-5.510664	-3.715368	-1.996115
1	-4.030794	-4.204008	-2.846827
1	-2.360242	-0.834211	-2.880394
6	-3.269563	-3.542840	2.132880
1	-2.437163	-2.872787	2.405500
1	-2.834858	-4.503922	1.818126
6	-4.817254	-1.662316	1.614413
1	-5.472931	-1.160597	0.887348
1	-4.058446	-0.931972	1.930921
1	-5.430925	-1.907518	2.501828
6	-5.261093	-3.940285	0.681491
1	-5.796262	-4.267829	1.593303
1	-4.854270	-4.842969	0.198466
1	-6.013253	-3.507479	0.005049
1	-5.199473	-3.129821	-3.642894
6	-2.960669	-1.697746	-3.197916
1	-3.472604	-1.428837	-4.141120
1	-2.251891	-2.508604	-3.429093
6	-4.161956	-2.927610	1.038373
1	-3.859563	-3.730945	3.049422
7	3.823910	-1.979493	-0.833475
7	2.805273	-2.414599	1.017065
6	2.792939	-1.571324	-0.047954

6	4.474303	-3.085859	-0.279864
6	3.830395	-3.357881	0.899832
6	4.095463	-1.338679	-2.133184
1	3.512866	-0.406381	-2.086003
6	3.534445	-2.171774	-3.285025
1	4.040681	-3.145820	-3.370136
1	2.457644	-2.344013	-3.138898
1	3.669878	-1.634913	-4.236468
6	5.562450	-0.951074	-2.318331
1	5.966808	-0.488879	-1.406212
1	6.195557	-1.807119	-2.589086
1	5.638722	-0.213691	-3.131102
6	1.807007	-2.317484	2.098459
1	1.257948	-1.393648	1.860994
6	0.791572	-3.454164	2.026077
1	-0.032823	-3.254497	2.726471
1	0.360581	-3.516523	1.017564
1	1.227384	-4.431485	2.283873
6	2.432603	-2.142473	3.481266
1	3.216966	-1.373273	3.464030
1	1.651521	-1.808843	4.181145
1	2.856932	-3.074355	3.881633
6	5.648729	-3.785522	-0.879585
1	6.572842	-3.190200	-0.807177
1	5.826155	-4.732489	-0.352461
1	5.490945	-4.024065	-1.941681
6	4.150097	-4.409841	1.909284
1	4.623774	-3.988357	2.810416
1	3.255196	-4.959103	2.233631
1	4.850420	-5.139689	1.481150
6	3.503325	3.235532	-0.996132
6	3.641977	4.737826	-0.693030
1	4.296982	5.223094	-1.441882
1	2.669554	5.252750	-0.730455
1	4.079769	4.928022	0.296579
6	4.898011	2.593403	-1.006746
1	5.437733	2.760658	-0.062889
1	4.843971	1.506271	-1.170903

1	1.904868	3.554175	-2.476169
6	3.815888	3.403752	2.551600
1	4.696279	3.682387	1.953168
1	3.119481	4.257456	2.542448
14	2.315485	2.323828	0.278670
6	0.862610	3.550826	0.553845
1	1.146306	4.398889	1.200123
1	0.516816	3.968307	-0.404352
1	0.000212	3.044040	1.012631
1	5.518240	3.019663	-1.817926
6	2.901465	3.092337	-2.404938
1	3.546331	3.590935	-3.153121
1	2.793715	2.036458	-2.701185
6	3.156340	2.112758	2.041187
6	2.039992	1.717123	3.024119
1	1.332332	2.544840	3.186397
1	1.458802	0.852807	2.662934
1	2.466581	1.453324	4.010061
6	4.204957	0.988912	2.021013
1	4.597826	0.806661	3.039736
1	3.774633	0.049599	1.648560
1	5.064722	1.230462	1.379614
1	4.162109	3.274867	3.595056

Table S6

B3LYP-D3(BJ)/def2-SVP

Rea-TlTl

Atomic Number	Coordinates (Angstroms) X	Y	Z
81	-1.375500	-0.706357	0.609004
81	1.332630	0.069128	-1.009712
7	-2.880454	2.551680	0.876561
7	-2.331305	2.352725	-1.192747
6	-2.485936	1.641500	-0.049591
6	-2.973451	3.833437	0.324723
6	-2.628433	3.704900	-0.995528
6	-3.227440	2.134217	2.244829
1	-2.968889	1.065419	2.255016
6	-2.374268	2.821577	3.309678
1	-2.622875	3.886262	3.422280
1	-1.306116	2.735082	3.067119
1	-2.544538	2.336925	4.282994
6	-4.731094	2.241380	2.503205
1	-5.296527	1.734006	1.709762
1	-5.067702	3.287198	2.558717
1	-4.979195	1.759394	3.460930
6	-1.998447	1.683654	-2.462847
1	-1.689784	0.676983	-2.147275
6	-0.808361	2.314552	-3.182547
1	-0.429973	1.608199	-3.936166
1	0.011033	2.519811	-2.480350
1	-1.071495	3.246834	-3.700870
6	-3.236151	1.540556	-3.348734
1	-4.046954	1.043108	-2.798572
1	-2.995352	0.930472	-4.232468
1	-3.602346	2.516838	-3.702476
6	-3.293523	5.078674	1.082115
1	-4.178874	4.966793	1.723744
1	-3.495297	5.901321	0.382980
1	-2.453139	5.391458	1.723492

6	-2.512003	4.773331	-2.030698
1	-3.007127	4.497831	-2.973176
1	-1.460357	5.006993	-2.262966
1	-2.981668	5.697732	-1.668596
14	-3.512507	-2.447368	0.008411
6	-3.375024	-3.894983	1.261844
1	-4.247228	-4.570415	1.226417
1	-3.282748	-3.524726	2.295492
1	-2.479223	-4.502709	1.054338
6	-3.244727	-3.280086	-1.745130
6	-3.604237	-2.306336	-2.876482
1	-3.323724	-2.728024	-3.859922
1	-3.074908	-1.346377	-2.765411
1	-4.683549	-2.091536	-2.909738
6	-4.055644	-4.576788	-1.906097
1	-5.139717	-4.401032	-1.854855
1	-3.801409	-5.315823	-1.130486
1	-1.110070	-2.728489	-1.849568
6	-5.403233	-1.379992	1.787274
1	-4.572764	-0.739884	2.128970
1	-5.388369	-2.294899	2.399224
6	-5.477066	-0.386198	-0.503882
1	-5.480037	-0.559980	-1.590425
1	-4.667266	0.326849	-0.288063
1	-6.440369	0.094986	-0.247776
6	-6.429295	-2.665210	-0.094720
1	-7.412830	-2.249332	0.196904
1	-6.325939	-3.641547	0.405420
1	-6.464295	-2.845604	-1.179820
1	-3.844464	-5.045992	-2.886239
6	-1.747629	-3.627491	-1.862951
1	-1.548502	-4.156365	-2.813834
1	-1.409790	-4.286998	-1.046946
6	-5.299555	-1.694257	0.282994
1	-6.346170	-0.846835	2.010569
7	4.358140	-1.865164	-0.499439
7	2.991375	-2.553594	1.010194
6	3.145508	-1.608027	0.050954

6	4.964422	-2.977611	0.095721
6	4.093391	-3.413555	1.061073
6	4.862813	-1.048014	-1.614636
1	4.182780	-0.184238	-1.622659
6	4.711670	-1.774322	-2.951222
1	5.359003	-2.663012	-3.011431
1	3.668584	-2.092773	-3.095359
1	4.985556	-1.101526	-3.778486
6	6.271448	-0.507252	-1.369105
1	6.353825	-0.082486	-0.358034
1	7.047474	-1.274877	-1.494552
1	6.481542	0.295913	-2.090725
6	1.772241	-2.598735	1.833411
1	1.244853	-1.677640	1.551271
6	0.866111	-3.766872	1.447253
1	-0.097330	-3.677290	1.971812
1	0.662850	-3.752571	0.366360
1	1.301629	-4.743265	1.709423
6	2.058891	-2.506796	3.331063
1	2.760411	-1.686298	3.541936
1	1.118828	-2.290406	3.861069
1	2.466679	-3.439106	3.747460
6	6.305184	-3.526968	-0.264066
1	7.129017	-2.888521	0.094039
1	6.437825	-4.518175	0.190617
1	6.426906	-3.644301	-1.350993
6	4.257115	-4.545332	2.020567
1	4.471148	-4.195278	3.043392
1	3.360097	-5.179350	2.070416
1	5.096179	-5.182805	1.710186
6	3.458873	3.505611	-0.637946
6	3.431135	4.981463	-0.205196
1	4.114519	5.583690	-0.834735
1	2.425331	5.417863	-0.306945
1	3.744873	5.114879	0.839799
6	4.897791	2.979473	-0.551337
1	5.320236	3.095900	0.458343
1	4.952445	1.911142	-0.811444

1	1.962608	3.768740	-2.234219
6	3.358670	3.353878	2.929662
1	4.275356	3.740594	2.459076
1	2.606668	4.158959	2.910991
14	2.225224	2.384760	0.408315
6	0.661675	3.485499	0.595399
1	0.818622	4.350964	1.262439
1	0.345274	3.878741	-0.383877
1	-0.180652	2.899207	0.987067
1	5.560733	3.525694	-1.249235
6	3.003955	3.430039	-2.107012
1	3.637112	4.073817	-2.746838
1	3.065106	2.403109	-2.503206
6	2.855709	2.074088	2.243446
6	1.660225	1.529648	3.045422
1	0.874536	2.290905	3.171567
1	1.193116	0.658600	2.557124
1	1.981041	1.219589	4.057879
6	3.971942	1.017603	2.268754
1	4.276588	0.799624	3.310654
1	3.639920	0.078023	1.805206
1	4.870970	1.349268	1.727352
1	3.598939	3.155733	3.992147

Table S7

B3LYP-D3(BJ)/def2-SVP

TS-BB

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.607697	2.341603	0.195383
5	0.744385	0.314949	-0.239537
7	2.420324	-0.994248	1.362051
7	2.964531	-1.261183	-0.721628
6	0.372931	0.816420	-2.130522
1	-0.433297	1.464758	-1.786816
1	1.155538	1.499450	-2.491784
6	0.117443	-0.233623	-3.066131
1	-0.388034	-1.154046	-2.780759
1	0.649309	-0.261571	-4.022030
14	-1.615559	-2.397362	0.181167
5	-0.824630	-0.376931	0.023866
6	2.035357	-0.646306	0.085531
6	3.520784	-1.847445	1.343116
6	3.867795	-2.010752	0.033784
6	1.748637	-0.537560	2.594917
1	1.144590	0.308353	2.253406
6	2.723469	-0.063275	3.680813
1	2.214274	0.675165	4.316107
1	3.616545	0.416689	3.260796
1	3.048263	-0.885439	4.331802
6	0.795135	-1.587005	3.144892
1	0.059210	-1.849164	2.384157
1	0.265883	-1.183003	4.021282
1	1.314964	-2.503145	3.461717
6	4.157288	-2.480330	2.536202
1	3.412535	-2.885455	3.234415
1	4.799668	-1.784858	3.097225
1	4.787887	-3.317725	2.210467
6	4.996379	-2.824794	-0.506478
1	5.356773	-3.510258	0.271667

1	5.849656	-2.201903	-0.815544
1	4.698191	-3.434115	-1.368900
6	3.010772	-1.194851	-2.199623
1	2.287494	-0.417704	-2.450187
6	4.390804	-0.803112	-2.743247
1	5.052610	-1.669440	-2.875363
1	4.897071	-0.069080	-2.105280
1	4.256834	-0.344976	-3.734199
6	2.492446	-2.472823	-2.852189
1	3.080750	-3.361988	-2.581482
1	2.536066	-2.354224	-3.944980
1	1.447785	-2.643100	-2.584240
6	2.084024	2.695258	2.023731
1	1.241582	2.720719	2.726150
1	2.567335	3.680218	2.076392
1	2.811413	1.974395	2.401049
6	3.418457	2.628371	-0.616675
6	3.940676	4.061019	-0.381942
1	3.364063	4.814775	-0.933898
1	4.983945	4.129929	-0.742791
1	3.950188	4.346592	0.679687
6	4.439013	1.695286	0.068588
1	4.175055	0.636102	0.000167
1	4.560358	1.939256	1.134484
1	5.433687	1.816575	-0.400343
6	3.472322	2.400765	-2.135511
1	3.151072	1.398083	-2.423515
1	4.506123	2.537487	-2.504567
1	2.836791	3.113920	-2.677822
6	0.515362	3.955038	-0.218959
6	-0.940182	3.687443	0.175245
1	-1.359399	2.854886	-0.385311
1	-1.567087	4.577273	-0.022847
1	-1.038958	3.453427	1.244022
6	0.941849	5.190131	0.603243
1	0.309524	6.049410	0.311010
1	1.984596	5.488688	0.447590
1	0.792176	5.036938	1.681946

6	0.565936	4.345119	-1.707841
1	0.340662	3.506063	-2.377429
1	1.551973	4.738417	-1.993009
1	-0.169419	5.145287	-1.915475
7	-2.628793	0.992797	1.344569
7	-2.893892	1.260250	-0.797353
6	-2.105533	0.608659	0.134766
6	-3.677549	1.893929	1.184255
6	-3.841887	2.062163	-0.160583
6	-2.089346	0.532687	2.636716
1	-1.460822	-0.318471	2.350173
6	-3.171202	0.046638	3.605176
1	-2.720151	-0.656949	4.320064
1	-3.981314	-0.479592	3.082630
1	-3.610145	0.868377	4.186804
6	-1.182091	1.577834	3.270764
1	-0.389557	1.851865	2.570577
1	-0.718643	1.166973	4.180772
1	-1.727388	2.490328	3.553824
6	-4.435425	2.548852	2.290469
1	-3.770898	2.949534	3.068747
1	-5.147180	1.864737	2.777672
1	-5.014458	3.390369	1.888360
6	-4.810266	2.960833	-0.854163
1	-5.201861	3.699451	-0.142179
1	-5.671357	2.414135	-1.268076
1	-4.335806	3.512010	-1.675807
6	-2.826813	1.119106	-2.271512
1	-2.059710	0.347649	-2.429864
6	-4.143261	0.625038	-2.880676
1	-4.867761	1.438694	-3.020324
1	-4.613326	-0.163554	-2.287170
1	-3.924204	0.210965	-3.876210
6	-2.349043	2.377071	-3.011215
1	-3.186168	2.965517	-3.416796
1	-1.715073	2.054268	-3.852550
1	-1.742649	3.032953	-2.381474
6	-2.269204	-2.807230	1.949476

1	-1.489199	-2.924082	2.712511
1	-2.817996	-3.758680	1.911303
1	-2.975125	-2.052974	2.307963
6	-3.312692	-2.682044	-0.825371
6	-3.873255	-4.112475	-0.683227
1	-3.231007	-4.870378	-1.149470
1	-4.853572	-4.168660	-1.192416
1	-4.040960	-4.404582	0.363891
6	-4.399637	-1.761407	-0.231001
1	-4.131817	-0.701275	-0.234954
1	-4.630810	-2.038355	0.808562
1	-5.339655	-1.865866	-0.804489
6	-3.149517	-2.423339	-2.332884
1	-2.615058	-1.493874	-2.552332
1	-4.134827	-2.382280	-2.831178
1	-2.584468	-3.230175	-2.815433
6	-0.465680	-3.970063	-0.203009
6	0.980646	-3.712697	0.225638
1	1.416620	-2.888214	-0.335539
1	1.600603	-4.609110	0.036467
1	1.062474	-3.482471	1.295165
6	-0.922659	-5.220458	0.576355
1	-0.291746	-6.080695	0.283866
1	-1.964979	-5.502555	0.386837
1	-0.802924	-5.089374	1.662152
6	-0.459593	-4.310860	-1.704730
1	-0.304390	-3.425310	-2.336776
1	-1.399960	-4.778056	-2.025234
1	0.350972	-5.028002	-1.930977

Table S8

B3LYP-D3(BJ)/def2-SVP

TS-AlAl

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-2.835281	-2.018767	0.404810
13	-1.089452	-0.255990	-0.280022
7	-2.248619	2.120400	1.192523
7	-2.464464	2.536931	-0.916485
6	-1.520244	-1.068601	-2.931649
1	-1.475758	-2.146205	-2.787548
1	-2.510673	-0.616934	-2.880372
6	-0.404010	-0.369022	-3.286314
1	-0.415868	0.692200	-3.532862
1	0.542195	-0.865150	-3.482174
14	2.797362	2.096628	0.360564
13	1.394879	0.306446	-0.732975
6	-2.120121	1.553671	-0.040984
6	-2.641851	3.454091	1.093492
6	-2.784208	3.718775	-0.243889
6	-1.882817	1.388407	2.419787
1	-1.769463	0.348037	2.080215
6	-2.992453	1.401794	3.468905
1	-2.771173	0.643349	4.234048
1	-3.965222	1.158745	3.018900
1	-3.071430	2.369537	3.982091
6	-0.526077	1.838029	2.951111
1	0.238140	1.710346	2.171689
1	-0.241859	1.220863	3.815792
1	-0.534332	2.888265	3.276502
6	-2.845575	4.380160	2.245889
1	-1.987984	4.377639	2.933908
1	-3.744443	4.128894	2.830513
1	-2.965153	5.407398	1.878531
6	-3.128068	5.015124	-0.897099
1	-3.484072	5.728782	-0.143021

1	-3.920794	4.912794	-1.651138
1	-2.251403	5.464336	-1.390622
6	-2.540936	2.299224	-2.367989
1	-2.190619	1.269980	-2.471505
6	-3.984495	2.335024	-2.874715
1	-4.394073	3.354921	-2.911879
1	-4.636850	1.720920	-2.237457
1	-4.021928	1.925947	-3.895662
6	-1.587396	3.183185	-3.170040
1	-1.888053	4.240031	-3.167348
1	-1.583797	2.844734	-4.217192
1	-0.562460	3.104107	-2.781985
6	-2.911092	-2.126919	2.324088
1	-1.958231	-2.465802	2.754221
1	-3.685023	-2.844516	2.639646
1	-3.159273	-1.163008	2.786327
6	-4.708367	-1.670549	-0.080686
6	-5.635080	-2.838472	0.296996
1	-5.413108	-3.749145	-0.277952
1	-6.690212	-2.574359	0.093246
1	-5.565825	-3.092437	1.366418
6	-5.167052	-0.421266	0.694966
1	-4.507841	0.440733	0.505626
1	-5.191988	-0.596501	1.781541
1	-6.189991	-0.132863	0.388442
6	-4.854892	-1.371428	-1.579316
1	-4.276072	-0.478761	-1.856460
1	-5.912279	-1.170538	-1.835003
1	-4.512390	-2.200943	-2.214314
6	-2.240159	-3.827116	-0.122857
6	-0.701464	-3.808084	-0.186394
1	-0.326161	-3.114359	-0.952354
1	-0.305684	-4.813818	-0.424045
1	-0.249944	-3.498742	0.769078
6	-2.660124	-4.878254	0.921811
1	-2.338120	-5.885460	0.596513
1	-3.750777	-4.913327	1.064567
1	-2.200997	-4.692697	1.904013

6	-2.788814	-4.281944	-1.485682
1	-2.563535	-3.577879	-2.297301
1	-3.879658	-4.418500	-1.464146
1	-2.345994	-5.256030	-1.766096
7	2.338615	-2.045501	1.196021
7	2.605158	-2.546673	-0.886485
6	2.227583	-1.527133	-0.061096
6	2.746111	-3.379830	1.160535
6	2.916292	-3.697467	-0.162443
6	2.031639	-1.246962	2.396104
1	1.897683	-0.233270	1.985711
6	3.187686	-1.209323	3.393432
1	3.000499	-0.409918	4.125925
1	4.136269	-0.985502	2.886168
1	3.298712	-2.147064	3.955493
6	0.702907	-1.660823	3.016792
1	-0.099470	-1.523430	2.279820
1	0.482026	-1.026715	3.888475
1	0.694983	-2.707764	3.353949
6	2.944386	-4.258749	2.351127
1	2.085725	-4.231265	3.037327
1	3.839681	-3.982746	2.930222
1	3.069442	-5.300263	2.026996
6	3.289537	-5.013802	-0.758440
1	3.602822	-5.707244	0.032768
1	4.121904	-4.933882	-1.472234
1	2.441035	-5.476171	-1.287666
6	2.775515	-2.344824	-2.337264
1	2.401814	-1.310595	-2.472751
6	4.250103	-2.356861	-2.737492
1	4.697704	-3.361508	-2.690723
1	4.831029	-1.684537	-2.090597
1	4.349833	-1.997417	-3.773263
6	1.905457	-3.275042	-3.178785
1	2.254723	-4.317649	-3.163481
1	1.925145	-2.938477	-4.226511
1	0.861412	-3.254486	-2.836495
6	3.007010	2.423784	2.251703

1	2.094392	2.860009	2.685612
1	3.830566	3.129595	2.451786
1	3.226159	1.501979	2.809020
6	4.655767	1.759323	-0.225285
6	5.585000	2.960229	0.014428
1	5.323039	3.812911	-0.629642
1	6.633660	2.690006	-0.216024
1	5.561016	3.309224	1.058972
6	5.181375	0.568490	0.598269
1	4.549531	-0.324095	0.469255
1	5.226193	0.798443	1.674423
1	6.206360	0.298897	0.279203
6	4.732504	1.376132	-1.712074
1	4.072706	0.528057	-1.949929
1	5.768026	1.094438	-1.985828
1	4.430002	2.203087	-2.369609
6	2.128384	3.824731	-0.311483
6	0.618143	3.854552	-0.027499
1	0.104903	3.002599	-0.496199
1	0.161143	4.782660	-0.422649
1	0.401178	3.822110	1.051071
6	2.764120	5.041851	0.379798
1	2.331682	5.980191	-0.018959
1	3.850917	5.091869	0.224639
1	2.584343	5.038645	1.466204
6	2.335974	3.939091	-1.829419
1	1.962902	3.043459	-2.353056
1	3.399528	4.056606	-2.086986
1	1.803264	4.823361	-2.231144

Table S9

B3LYP-D3(BJ)/def2-SVP

TS-GaGa

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-3.452514	-1.207874	0.501207
31	-1.228079	-0.105844	-0.211422
7	-1.693226	2.661743	1.092774
7	-1.688866	2.998746	-1.038395
6	-1.381353	-0.932102	-2.799689
1	-1.509599	-1.978635	-2.522757
1	-2.280167	-0.311757	-2.754314
6	-0.224425	-0.503748	-3.372857
1	-0.089667	0.515918	-3.733633
1	0.592138	-1.186587	-3.594912
14	3.337104	1.375585	0.582629
31	1.578610	0.059298	-0.893709
6	-1.734163	2.014381	-0.103769
6	-1.611042	4.044747	0.914547
6	-1.616006	4.260121	-0.438117
6	-1.625559	1.915464	2.361134
1	-1.872832	0.884710	2.070533
6	-2.687972	2.354034	3.367538
1	-2.743153	1.611617	4.177403
1	-3.677565	2.414284	2.892808
1	-2.454948	3.323683	3.827709
6	-0.208039	1.912312	2.928986
1	0.503195	1.529065	2.184373
1	-0.162958	1.266382	3.817417
1	0.116200	2.917797	3.233444
6	-1.519097	5.051050	2.012214
1	-0.721531	4.806161	2.728516
1	-2.460198	5.143896	2.576795
1	-1.285039	6.037438	1.591824
6	-1.491632	5.556334	-1.166358
1	-1.645010	6.391165	-0.470270

1	-2.232165	5.660276	-1.971400
1	-0.491270	5.676954	-1.612192
6	-1.734893	2.699268	-2.479779
1	-1.721988	1.605401	-2.508435
6	-3.046671	3.160176	-3.117489
1	-3.105542	4.254448	-3.210544
1	-3.909176	2.813814	-2.530298
1	-3.130210	2.736611	-4.129861
6	-0.488370	3.184569	-3.218446
1	-0.430059	4.280175	-3.272768
1	-0.512151	2.806001	-4.251401
1	0.421118	2.800201	-2.735415
6	-3.657158	-1.227409	2.411528
1	-2.879394	-1.839421	2.893019
1	-4.633323	-1.651566	2.698782
1	-3.601232	-0.220059	2.846959
6	-5.072169	-0.318126	-0.154333
6	-6.344347	-1.141335	0.105861
1	-6.353321	-2.083599	-0.461141
1	-7.242922	-0.570707	-0.196689
1	-6.462385	-1.390732	1.172455
6	-5.202522	1.024227	0.589199
1	-4.301438	1.644757	0.464932
1	-5.373070	0.883116	1.667891
1	-6.061115	1.599425	0.195154
6	-4.955842	-0.016766	-1.656927
1	-4.083405	0.621527	-1.862648
1	-5.851542	0.522965	-2.017792
1	-4.852672	-0.927127	-2.264669
6	-3.392367	-3.117537	0.019122
6	-1.935639	-3.595562	0.174665
1	-1.244983	-3.082584	-0.511502
1	-1.858866	-4.681639	-0.022388
1	-1.557674	-3.423102	1.193686
6	-4.270328	-3.964973	0.959003
1	-4.229945	-5.029428	0.659649
1	-5.326735	-3.658840	0.935688
1	-3.930078	-3.909478	2.004049

6	-3.847923	-3.380599	-1.425944
1	-3.299980	-2.776123	-2.161640
1	-4.919829	-3.174933	-1.562864
1	-3.686975	-4.442981	-1.689040
7	1.534939	-2.576464	1.215851
7	1.944965	-3.192628	-0.806757
6	1.845037	-2.090748	-0.016353
6	1.426697	-3.970715	1.200163
6	1.694924	-4.362512	-0.085189
6	1.426275	-1.690960	2.387656
1	1.592850	-0.691325	1.959962
6	2.538129	-1.950473	3.404714
1	2.516641	-1.166020	4.175765
1	3.521884	-1.921144	2.917784
1	2.427987	-2.917370	3.916668
6	0.030706	-1.715116	3.002254
1	-0.721537	-1.473128	2.240206
1	-0.034278	-0.962730	3.801001
1	-0.222444	-2.688342	3.445528
6	1.009555	-4.826527	2.350038
1	-0.067000	-4.725404	2.564000
1	1.555873	-4.594358	3.274016
1	1.194647	-5.883065	2.114271
6	1.675152	-5.741187	-0.656404
1	1.661464	-6.481727	0.154493
1	2.558641	-5.948106	-1.277356
1	0.782261	-5.917588	-1.277969
6	2.374394	-3.085038	-2.210660
1	2.311563	-2.001045	-2.403029
6	3.833228	-3.508607	-2.379371
1	3.977380	-4.585529	-2.199574
1	4.478114	-2.950953	-1.685152
1	4.168618	-3.291483	-3.405286
6	1.419837	-3.780892	-3.180824
1	1.519610	-4.875076	-3.168543
1	1.637047	-3.444625	-4.205854
1	0.375179	-3.522625	-2.954493
6	3.459570	1.594060	2.494630

1	2.657077	2.248154	2.869714
1	4.418652	2.054024	2.789283
1	3.378767	0.636498	3.028030
6	5.077455	0.590184	0.088626
6	6.269089	1.521287	0.357595
1	6.255123	2.403717	-0.299790
1	7.225734	0.994569	0.173223
1	6.290113	1.879717	1.399316
6	5.252592	-0.685742	0.932677
1	4.409920	-1.380435	0.785064
1	5.325502	-0.463025	2.008932
1	6.179935	-1.217108	0.644935
6	5.095229	0.175648	-1.392469
1	4.273630	-0.518831	-1.628433
1	6.045947	-0.334056	-1.642653
1	4.993269	1.035098	-2.070214
6	3.164846	3.232300	-0.061944
6	1.696454	3.634946	0.160216
1	1.002653	2.953164	-0.353805
1	1.507304	4.657573	-0.219959
1	1.428612	3.633846	1.227777
6	4.049933	4.238518	0.691331
1	3.871761	5.266250	0.318056
1	5.121721	4.028616	0.567351
1	3.836327	4.244658	1.771691
6	3.464473	3.325141	-1.566368
1	2.885617	2.586030	-2.143906
1	4.530277	3.156191	-1.783538
1	3.209260	4.331127	-1.953464

Table S10

B3LYP-D3(BJ)/def2-SVP

TS-InIn

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-3.701984	-0.837252	0.607435
49	-1.253422	-0.019250	-0.264596
7	-1.414523	3.035397	1.058454
7	-1.217099	3.341979	-1.064354
6	-1.400553	-0.633450	-2.887883
1	-1.771917	-1.648499	-2.727113
1	-2.172910	0.137036	-2.976700
6	-0.125272	-0.433694	-3.383417
1	0.203514	0.536280	-3.757864
1	0.523335	-1.268581	-3.640064
14	3.574947	0.977443	0.697342
49	1.638357	-0.137217	-0.915008
6	-1.504657	2.395078	-0.137026
6	-1.063696	4.377566	0.887957
6	-0.949898	4.575481	-0.463517
6	-1.575636	2.299477	2.324471
1	-2.016184	1.343322	2.008873
6	-2.575806	2.952828	3.277046
1	-2.839572	2.233447	4.066857
1	-3.499497	3.228704	2.748740
1	-2.167717	3.845465	3.770359
6	-0.223948	2.002236	2.973166
1	0.440692	1.485963	2.266168
1	-0.367200	1.355028	3.850861
1	0.279964	2.918945	3.313372
6	-0.843299	5.358076	1.990732
1	-0.146892	4.971390	2.749320
1	-1.778517	5.632637	2.503713
1	-0.402798	6.278574	1.586359
6	-0.559177	5.820003	-1.187885
1	-0.615829	6.681421	-0.509531

1	-1.218157	6.030473	-2.042260
1	0.473804	5.763164	-1.567027
6	-1.245270	3.028636	-2.503635
1	-1.350032	1.938912	-2.518392
6	-2.480994	3.621919	-3.180941
1	-2.446086	4.721273	-3.220274
1	-3.395147	3.322489	-2.647357
1	-2.550446	3.252155	-4.215353
6	0.066091	3.362166	-3.213328
1	0.223762	4.442829	-3.331381
1	0.047508	2.921481	-4.221245
1	0.921437	2.931513	-2.673661
6	-3.895328	-0.820621	2.517666
1	-3.225016	-1.559210	2.985361
1	-4.925316	-1.066988	2.826557
1	-3.650488	0.161437	2.949666
6	-5.156181	0.277785	-0.081784
6	-6.540754	-0.358764	0.117519
1	-6.662293	-1.279748	-0.471823
1	-7.338437	0.339127	-0.200909
1	-6.730543	-0.609064	1.173799
6	-5.115964	1.614861	0.680754
1	-4.133974	2.103092	0.579819
1	-5.327954	1.487019	1.753838
1	-5.875230	2.310426	0.276883
6	-4.938154	0.581073	-1.574063
1	-3.979077	1.098148	-1.734583
1	-5.738889	1.240647	-1.958299
1	-4.933008	-0.327051	-2.194120
6	-3.891458	-2.731821	0.118873
6	-2.531130	-3.411906	0.364133
1	-1.738340	-3.009680	-0.286006
1	-2.597446	-4.499439	0.171115
1	-2.191651	-3.286478	1.404002
6	-4.946619	-3.445577	0.982672
1	-5.029663	-4.508732	0.686735
1	-5.945501	-2.997634	0.877260
1	-4.684405	-3.425989	2.051681

6	-4.261516	-2.908763	-1.362013
1	-3.562300	-2.384798	-2.030473
1	-5.273124	-2.536881	-1.582920
1	-4.241753	-3.979750	-1.638642
7	1.175306	-2.865642	1.243079
7	1.428887	-3.551528	-0.781362
6	1.557380	-2.451538	0.005455
6	0.804544	-4.214288	1.237107
6	0.971308	-4.651915	-0.051037
6	1.227788	-1.961455	2.404942
1	1.545021	-1.004701	1.965318
6	2.299786	-2.389051	3.407927
1	2.406383	-1.615399	4.182694
1	3.270899	-2.507282	2.908952
1	2.048916	-3.331402	3.916053
6	-0.141707	-1.751126	3.046967
1	-0.878448	-1.436687	2.295201
1	-0.069379	-0.957871	3.804816
1	-0.518363	-2.653462	3.548722
6	0.267347	-4.976559	2.402786
1	-0.763599	-4.675558	2.648768
1	0.876313	-4.851093	3.308396
1	0.243744	-6.048937	2.167163
6	0.679629	-6.002236	-0.615629
1	0.547132	-6.727281	0.198567
1	1.492871	-6.370999	-1.257255
1	-0.245901	-6.007425	-1.213990
6	1.833206	-3.522619	-2.196980
1	1.968624	-2.447115	-2.392748
6	3.184501	-4.206173	-2.402326
1	3.139070	-5.288229	-2.202578
1	3.941722	-3.762400	-1.738843
1	3.518256	-4.070132	-3.442632
6	0.739316	-4.022741	-3.139871
1	0.625315	-5.115404	-3.122973
1	0.992501	-3.735815	-4.171522
1	-0.229085	-3.564820	-2.890766
6	3.546709	1.093074	2.619092

1	2.738679	1.759622	2.959826
1	4.494209	1.492951	3.020170
1	3.382269	0.112762	3.087510
6	5.247155	0.023089	0.288684
6	6.510026	0.805188	0.679788
1	6.643424	1.703230	0.057619
1	7.414362	0.180456	0.545420
1	6.489671	1.127298	1.733406
6	5.214710	-1.293739	1.086502
1	4.305971	-1.875980	0.860047
1	5.245110	-1.119430	2.173521
1	6.088010	-1.923389	0.830857
6	5.325219	-0.339170	-1.204228
1	4.464297	-0.952322	-1.517687
1	6.242612	-0.921868	-1.414470
1	5.342921	0.549063	-1.852401
6	3.625637	2.865141	0.136077
6	2.199228	3.416387	0.311816
1	1.462381	2.857180	-0.284382
1	2.148039	4.476178	-0.003402
1	1.868684	3.375681	1.361035
6	4.574392	3.734775	0.977193
1	4.525723	4.791098	0.647561
1	5.622387	3.414807	0.891439
1	4.308088	3.716116	2.045658
6	4.008751	2.986920	-1.346816
1	3.381414	2.342322	-1.984570
1	5.058851	2.708112	-1.524254
1	3.884704	4.029746	-1.698278

Table S11

B3LYP-D3(BJ)/def2-SVP

TS-TlTl

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-3.937102	-0.676970	0.598430
81	-1.410827	-0.096737	-0.299404
7	-1.274582	3.065418	1.155824
7	-1.080997	3.428260	-0.954415
6	-1.042117	-0.516331	-2.849548
1	-1.452637	-1.531806	-2.882945
1	-1.745864	0.242683	-3.210566
6	0.342340	-0.347409	-3.118015
1	0.696195	0.598822	-3.534580
1	0.945446	-1.205526	-3.420754
14	3.707913	0.882501	0.778203
81	1.563334	-0.068685	-0.697086
6	-1.440088	2.477384	-0.057314
6	-0.813292	4.380045	1.026788
6	-0.698528	4.613786	-0.318719
6	-1.474055	2.298527	2.396269
1	-1.948519	1.371042	2.047326
6	-2.451691	2.965865	3.362226
1	-2.729410	2.247184	4.148001
1	-3.370668	3.267080	2.838631
1	-2.022133	3.846791	3.859336
6	-0.138065	1.923404	3.038316
1	0.503903	1.403302	2.313356
1	-0.309765	1.253327	3.893497
1	0.405609	2.804063	3.410823
6	-0.510279	5.305174	2.157800
1	0.170791	4.850384	2.892222
1	-1.417638	5.621713	2.696412
1	-0.018095	6.209528	1.776917
6	-0.211353	5.843114	-1.010072
1	-0.170150	6.680875	-0.301435

1	-0.868863	6.144750	-1.838289
1	0.802100	5.706553	-1.420488
6	-1.154952	3.160285	-2.399852
1	-1.350741	2.082993	-2.439835
6	-2.343675	3.874474	-3.043295
1	-2.221602	4.968567	-3.043158
1	-3.273855	3.628198	-2.510307
1	-2.451335	3.549853	-4.089684
6	0.171334	3.406758	-3.118465
1	0.396733	4.475123	-3.241977
1	0.123360	2.961097	-4.123125
1	1.000987	2.930331	-2.576551
6	-4.228649	-0.575685	2.490129
1	-3.629262	-1.335284	3.017429
1	-5.286712	-0.743004	2.756651
1	-3.939773	0.407036	2.892417
6	-5.227742	0.541640	-0.224413
6	-6.674640	0.031306	-0.138417
1	-6.827373	-0.877842	-0.739626
1	-7.379096	0.795072	-0.519710
1	-6.971505	-0.197229	0.898095
6	-5.129947	1.883584	0.525479
1	-4.098743	2.271394	0.518487
1	-5.458027	1.796933	1.573315
1	-5.774134	2.641318	0.041402
6	-4.862225	0.794697	-1.697757
1	-3.849370	1.216532	-1.790080
1	-5.566949	1.515722	-2.153360
1	-4.892868	-0.123471	-2.302524
6	-4.226837	-2.560143	0.138716
6	-2.994939	-3.349335	0.623082
1	-2.067264	-3.026748	0.124009
1	-3.121454	-4.429126	0.417074
1	-2.841290	-3.240849	1.708711
6	-5.470884	-3.151161	0.824308
1	-5.581957	-4.222020	0.567130
1	-6.396966	-2.643970	0.518726
1	-5.402460	-3.086031	1.921691

6	-4.347823	-2.739719	-1.382605
1	-3.493681	-2.293089	-1.916672
1	-5.265762	-2.280329	-1.779568
1	-4.380267	-3.813678	-1.646274
7	1.009649	-2.929708	1.324315
7	1.430496	-3.608851	-0.671940
6	1.527839	-2.524190	0.136218
6	0.588308	-4.262568	1.269231
6	0.858508	-4.696402	-0.003055
6	1.004883	-2.034234	2.493194
1	1.333812	-1.072091	2.076656
6	2.042297	-2.467269	3.530045
1	2.110258	-1.710749	4.326185
1	3.033061	-2.565693	3.064821
1	1.782320	-3.426161	4.002910
6	-0.389948	-1.832648	3.082790
1	-1.105218	-1.541525	2.301458
1	-0.353793	-1.024580	3.827257
1	-0.769568	-2.729876	3.590320
6	-0.073197	-5.010734	2.378654
1	-1.112512	-4.680226	2.532295
1	0.458026	-4.900381	3.334596
1	-0.103805	-6.082394	2.140044
6	0.569377	-6.029017	-0.609893
1	0.315855	-6.751471	0.177594
1	1.430337	-6.431677	-1.163242
1	-0.284137	-5.989504	-1.306008
6	1.977610	-3.577192	-2.037833
1	2.190874	-2.511184	-2.193888
6	3.304410	-4.332437	-2.122291
1	3.177474	-5.413801	-1.959071
1	4.011073	-3.948458	-1.371611
1	3.751832	-4.193614	-3.118535
6	0.959770	-3.998875	-3.096924
1	0.780342	-5.082882	-3.105635
1	1.335057	-3.719081	-4.092670
1	0.001360	-3.482894	-2.941268
6	3.656410	0.914552	2.695407

1	2.897360	1.627542	3.053671
1	4.626512	1.217046	3.127500
1	3.404055	-0.071218	3.110831
6	5.274650	-0.196500	0.307575
6	6.605025	0.488382	0.656464
1	6.779793	1.382324	0.038390
1	7.455493	-0.198521	0.482266
1	6.646623	0.797898	1.713351
6	5.167599	-1.513198	1.100031
1	4.202508	-2.013774	0.915496
1	5.265130	-1.351099	2.185009
1	5.971891	-2.210711	0.799094
6	5.263805	-0.546234	-1.190746
1	4.352711	-1.101201	-1.467523
1	6.130360	-1.185016	-1.446258
1	5.312134	0.346631	-1.831584
6	3.859026	2.768388	0.260262
6	2.474275	3.405106	0.482341
1	1.692734	2.926576	-0.127111
1	2.492072	4.478421	0.214247
1	2.151896	3.339792	1.533110
6	4.883967	3.545803	1.102991
1	4.899318	4.612798	0.807588
1	5.905415	3.158353	0.980839
1	4.640933	3.509769	2.176642
6	4.216570	2.899611	-1.228111
1	3.526690	2.322526	-1.866265
1	5.237954	2.547504	-1.439747
1	4.162069	3.956680	-1.551457

Table S11

B3LYP-D3(BJ)/def2-SVP

Prod-BB

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-1.825561	2.684641	0.243682
5	-0.257432	1.440546	-0.312984
7	1.719881	2.232524	1.266690
7	2.219484	2.296399	-0.859025
6	-0.492533	0.585234	-1.664430
1	-1.511874	0.183841	-1.621205
1	-0.488780	1.157982	-2.619507
6	0.492533	-0.585234	-1.664430
1	1.511874	-0.183841	-1.621205
1	0.488780	-1.157982	-2.619507
14	1.825561	-2.684641	0.243682
5	0.257432	-1.440546	-0.312984
6	1.192560	1.964654	0.016266
6	3.038167	2.674589	1.171979
6	3.353336	2.717030	-0.155228
6	1.054907	1.813678	2.508042
1	0.024519	1.628896	2.192520
6	1.042920	2.893128	3.591361
1	0.241310	2.670451	4.310903
1	0.847623	3.886994	3.164485
1	1.984886	2.936353	4.154270
6	1.625414	0.484833	2.992568
1	1.506035	-0.261006	2.196964
1	1.087940	0.141482	3.887548
1	2.691156	0.559012	3.250829
6	3.909764	3.018491	2.333665
1	3.971562	2.201287	3.066738
1	3.556189	3.915404	2.865068
1	4.929595	3.221699	1.984013
6	4.678215	3.023411	-0.769203
1	5.371057	3.380007	0.003463

1	4.629564	3.799661	-1.545112
1	5.125083	2.124849	-1.223690
6	2.051513	2.464825	-2.315785
1	1.033544	2.121237	-2.502360
6	2.128302	3.937986	-2.737855
1	3.162570	4.307073	-2.783529
1	1.560394	4.579807	-2.054882
1	1.696182	4.049492	-3.743803
6	2.992649	1.590778	-3.148787
1	4.027415	1.959142	-3.138813
1	2.652500	1.600095	-4.195639
1	2.990544	0.550981	-2.802755
6	-2.051513	3.134715	2.091376
1	-2.288790	2.258127	2.712926
1	-2.882710	3.847268	2.202252
1	-1.162903	3.614317	2.516445
6	-1.509998	4.439043	-0.599335
6	-2.667968	5.432143	-0.405542
1	-3.576052	5.117258	-0.939418
1	-2.387791	6.425780	-0.804177
1	-2.929146	5.569500	0.655312
6	-0.258809	5.056139	0.056602
1	0.619939	4.400920	-0.010992
1	-0.424914	5.275776	1.122874
1	-0.000490	6.012893	-0.435010
6	-1.260552	4.285884	-2.108689
1	-0.502051	3.524823	-2.326016
1	-0.915545	5.240662	-2.547992
1	-2.172598	3.992913	-2.644849
6	-3.597212	2.000586	-0.261508
6	-3.697166	0.547045	0.223219
1	-2.899573	-0.077205	-0.187573
1	-4.665904	0.105283	-0.076798
1	-3.640002	0.480598	1.318686
6	-4.747411	2.773759	0.412229
1	-5.717591	2.347666	0.094050
1	-4.759483	3.840588	0.153045
1	-4.707185	2.696340	1.509077

6	-3.827476	2.035532	-1.783073
1	-2.989933	1.606317	-2.350926
1	-3.980676	3.061946	-2.148628
1	-4.737436	1.463345	-2.045292
7	-1.719881	-2.232524	1.266690
7	-2.219484	-2.296399	-0.859025
6	-1.192560	-1.964654	0.016266
6	-3.038167	-2.674589	1.171979
6	-3.353336	-2.717030	-0.155228
6	-1.054907	-1.813678	2.508042
1	-0.024519	-1.628896	2.192520
6	-1.042920	-2.893128	3.591361
1	-0.241310	-2.670451	4.310903
1	-0.847623	-3.886994	3.164485
1	-1.984886	-2.936353	4.154270
6	-1.625414	-0.484833	2.992568
1	-1.506035	0.261006	2.196964
1	-1.087940	-0.141482	3.887548
1	-2.691156	-0.559012	3.250829
6	-3.909764	-3.018491	2.333665
1	-3.971562	-2.201287	3.066738
1	-3.556189	-3.915404	2.865068
1	-4.929595	-3.221699	1.984013
6	-4.678215	-3.023411	-0.769203
1	-5.371057	-3.380007	0.003463
1	-4.629564	-3.799661	-1.545112
1	-5.125083	-2.124849	-1.223690
6	-2.051513	-2.464825	-2.315785
1	-1.033544	-2.121237	-2.502360
6	-2.128302	-3.937986	-2.737855
1	-3.162570	-4.307073	-2.783529
1	-1.560394	-4.579807	-2.054882
1	-1.696182	-4.049492	-3.743803
6	-2.992649	-1.590778	-3.148787
1	-4.027415	-1.959142	-3.138813
1	-2.652500	-1.600095	-4.195639
1	-2.990544	-0.550981	-2.802755
6	2.051513	-3.134715	2.091376

1	2.288790	-2.258127	2.712926
1	2.882710	-3.847268	2.202252
1	1.162903	-3.614317	2.516445
6	1.509998	-4.439043	-0.599335
6	2.667968	-5.432143	-0.405542
1	3.576052	-5.117258	-0.939418
1	2.387791	-6.425780	-0.804177
1	2.929146	-5.569500	0.655312
6	0.258809	-5.056139	0.056602
1	-0.619939	-4.400920	-0.010992
1	0.424914	-5.275776	1.122874
1	0.000490	-6.012893	-0.435010
6	1.260552	-4.285884	-2.108689
1	0.502051	-3.524823	-2.326016
1	0.915545	-5.240662	-2.547992
1	2.172598	-3.992913	-2.644849
6	3.597212	-2.000586	-0.261508
6	3.697166	-0.547045	0.223219
1	2.899573	0.077205	-0.187573
1	4.665904	-0.105283	-0.076798
1	3.640002	-0.480598	1.318686
6	4.747411	-2.773759	0.412229
1	5.717591	-2.347666	0.094050
1	4.759483	-3.840588	0.153045
1	4.707185	-2.696340	1.509077
6	3.827476	-2.035532	-1.783073
1	2.989933	-1.606317	-2.350926
1	3.980676	-3.061946	-2.148628
1	4.737436	-1.463345	-2.045292

Table S12

B3LYP-D3(BJ)/def2-SVP

Prod-AlAl

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-2.277161	2.691630	0.309705
13	-0.358078	1.254953	-0.398175
7	1.907469	2.443195	1.270846
7	2.389713	2.693468	-0.820102
6	-0.478358	0.611496	-2.329580
1	-1.523416	0.252405	-2.392659
1	-0.366841	1.281252	-3.207923
6	0.478358	-0.611496	-2.329580
1	1.523416	-0.252405	-2.392659
1	0.366841	-1.281252	-3.207923
14	2.277161	-2.691630	0.309705
13	0.358078	-1.254953	-0.398175
6	1.400020	2.278062	0.016683
6	3.213243	2.933006	1.223309
6	3.518051	3.094692	-0.103377
6	1.140721	2.060509	2.470520
1	0.137963	1.840645	2.077728
6	1.003295	3.211629	3.465823
1	0.223620	2.962123	4.200363
1	0.703968	4.137435	2.953391
1	1.931379	3.400887	4.022740
6	1.669761	0.769696	3.090866
1	1.617520	-0.043539	2.354860
1	1.048992	0.494467	3.956101
1	2.707077	0.866591	3.442191
6	4.073085	3.215683	2.410210
1	4.109361	2.367248	3.108409
1	3.728608	4.096614	2.974449
1	5.102275	3.413702	2.084093
6	4.805386	3.541350	-0.710484
1	5.462612	3.952585	0.066721

1	4.661860	4.324274	-1.468471
1	5.339841	2.706336	-1.190699
6	2.191419	2.769996	-2.280587
1	1.225076	2.274864	-2.429016
6	2.053309	4.220657	-2.745775
1	3.002396	4.773927	-2.677535
1	1.296913	4.750571	-2.150734
1	1.731051	4.238928	-3.798005
6	3.237299	1.980530	-3.068440
1	4.199125	2.507618	-3.145205
1	2.865380	1.819665	-4.091108
1	3.410462	0.993942	-2.618365
6	-2.496398	3.012856	2.188026
1	-2.760252	2.083072	2.716926
1	-3.298402	3.743347	2.384249
1	-1.578959	3.403440	2.649573
6	-2.062343	4.468992	-0.492877
6	-3.316100	5.349134	-0.380090
1	-4.152077	4.948734	-0.973127
1	-3.110720	6.369675	-0.756336
1	-3.661164	5.448608	0.661622
6	-0.907365	5.166215	0.251640
1	0.015255	4.564333	0.231033
1	-1.156342	5.362802	1.306666
1	-0.678047	6.141437	-0.217880
6	-1.669761	4.336014	-1.973584
1	-0.801311	3.673255	-2.102446
1	-1.411791	5.323428	-2.401341
1	-2.482775	3.916193	-2.582054
6	-3.961816	1.834085	-0.224593
6	-3.879882	0.358235	0.200826
1	-3.033687	-0.157294	-0.273868
1	-4.804603	-0.180374	-0.081442
1	-3.760908	0.246998	1.289223
6	-5.190524	2.458873	0.457570
1	-6.112342	1.932723	0.143195
1	-5.317533	3.520933	0.203468
1	-5.132561	2.383930	1.554600

6	-4.154134	1.883701	-1.748774
1	-3.270283	1.508185	-2.286595
1	-4.353387	2.905248	-2.106324
1	-5.019303	1.262028	-2.049151
7	-1.907469	-2.443195	1.270846
7	-2.389713	-2.693468	-0.820102
6	-1.400020	-2.278062	0.016683
6	-3.213243	-2.933006	1.223309
6	-3.518051	-3.094692	-0.103377
6	-1.140721	-2.060509	2.470520
1	-0.137963	-1.840645	2.077728
6	-1.003295	-3.211629	3.465823
1	-0.223620	-2.962123	4.200363
1	-0.703968	-4.137435	2.953391
1	-1.931379	-3.400887	4.022740
6	-1.669761	-0.769696	3.090866
1	-1.617520	0.043539	2.354860
1	-1.048992	-0.494467	3.956101
1	-2.707077	-0.866591	3.442191
6	-4.073085	-3.215683	2.410210
1	-4.109361	-2.367248	3.108409
1	-3.728608	-4.096614	2.974449
1	-5.102275	-3.413702	2.084093
6	-4.805386	-3.541350	-0.710484
1	-5.462612	-3.952585	0.066721
1	-4.661860	-4.324274	-1.468471
1	-5.339841	-2.706336	-1.190699
6	-2.191419	-2.769996	-2.280587
1	-1.225076	-2.274864	-2.429016
6	-2.053309	-4.220657	-2.745775
1	-3.002396	-4.773927	-2.677535
1	-1.296913	-4.750571	-2.150734
1	-1.731051	-4.238928	-3.798005
6	-3.237299	-1.980530	-3.068440
1	-4.199125	-2.507618	-3.145205
1	-2.865380	-1.819665	-4.091108
1	-3.410462	-0.993942	-2.618365
6	2.496398	-3.012856	2.188026

1	2.760252	-2.083072	2.716926
1	3.298402	-3.743347	2.384249
1	1.578959	-3.403440	2.649573
6	2.062343	-4.468992	-0.492877
6	3.316100	-5.349134	-0.380090
1	4.152077	-4.948734	-0.973127
1	3.110720	-6.369675	-0.756336
1	3.661164	-5.448608	0.661622
6	0.907365	-5.166215	0.251640
1	-0.015255	-4.564333	0.231033
1	1.156342	-5.362802	1.306666
1	0.678047	-6.141437	-0.217880
6	1.669761	-4.336014	-1.973584
1	0.801311	-3.673255	-2.102446
1	1.411791	-5.323428	-2.401341
1	2.482775	-3.916193	-2.582054
6	3.961816	-1.834085	-0.224593
6	3.879882	-0.358235	0.200826
1	3.033687	0.157294	-0.273868
1	4.804603	0.180374	-0.081442
1	3.760908	-0.246998	1.289223
6	5.190524	-2.458873	0.457570
1	6.112342	-1.932723	0.143195
1	5.317533	-3.520933	0.203468
1	5.132561	-2.383930	1.554600
6	4.154134	-1.883701	-1.748774
1	3.270283	-1.508185	-2.286595
1	4.353387	-2.905248	-2.106324
1	5.019303	-1.262028	-2.049151

Table S13

B3LYP-D3(BJ)/def2-SVP

Prod-GaGa

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-2.332023	2.595472	0.330595
31	-0.408050	1.212741	-0.356174
7	1.846569	2.479061	1.309236
7	2.314933	2.763993	-0.779484
6	-0.489440	0.595633	-2.330690
1	-1.525971	0.227097	-2.422678
1	-0.364320	1.303496	-3.175150
6	0.489440	-0.595633	-2.330690
1	1.525971	-0.227097	-2.422678
1	0.364320	-1.303496	-3.175150
14	2.332023	-2.595472	0.330595
31	0.408050	-1.212741	-0.356174
6	1.341768	2.313272	0.055877
6	3.138273	3.008015	1.263300
6	3.433896	3.192084	-0.061936
6	1.092730	2.070948	2.508523
1	0.095428	1.834210	2.115196
6	0.935141	3.209941	3.514915
1	0.160298	2.938714	4.246994
1	0.617819	4.134908	3.011656
1	1.858961	3.412318	4.074318
6	1.650378	0.785554	3.114413
1	1.611634	-0.020276	2.369982
1	1.039402	0.488680	3.979425
1	2.687379	0.899171	3.461923
6	3.994817	3.298699	2.450645
1	4.052703	2.443833	3.139589
1	3.632390	4.165402	3.025593
1	5.018258	3.523670	2.123672
6	4.706339	3.679796	-0.669079
1	5.355942	4.099418	0.110118

1	4.538963	4.467306	-1.417347
1	5.260687	2.864845	-1.161210
6	2.110794	2.844073	-2.238360
1	1.154882	2.329396	-2.383643
6	1.942055	4.293425	-2.697778
1	2.882221	4.862914	-2.640375
1	1.184191	4.809049	-2.092419
1	1.606518	4.308576	-3.745881
6	3.170499	2.080059	-3.032939
1	4.121587	2.626616	-3.108251
1	2.800088	1.917373	-4.055894
1	3.364474	1.094917	-2.588483
6	-2.555240	2.906648	2.208128
1	-2.800902	1.971510	2.735490
1	-3.371225	3.621359	2.404405
1	-1.645878	3.315297	2.669528
6	-2.147499	4.376875	-0.467419
6	-3.422530	5.226637	-0.352447
1	-4.248700	4.808937	-0.947125
1	-3.239819	6.252262	-0.726200
1	-3.770405	5.316387	0.689200
6	-1.011419	5.100523	0.280934
1	-0.073412	4.524060	0.256759
1	-1.265413	5.285230	1.336867
1	-0.809478	6.083923	-0.183817
6	-1.752337	4.259164	-1.948582
1	-0.866463	3.621544	-2.077982
1	-1.523529	5.255154	-2.372636
1	-2.553957	3.818706	-2.557505
6	-3.994817	1.705134	-0.208914
6	-3.885172	0.230946	0.214567
1	-3.030785	-0.266475	-0.262672
1	-4.800397	-0.323528	-0.066889
1	-3.762373	0.120802	1.302502
6	-5.235152	2.304981	0.475593
1	-6.146235	1.762486	0.158288
1	-5.382661	3.365340	0.226117
1	-5.176448	2.226030	1.572249

6	-4.189906	1.754065	-1.732939
1	-3.301357	1.393819	-2.273048
1	-4.406618	2.772617	-2.088519
1	-5.045142	1.118534	-2.032221
7	-1.846569	-2.479061	1.309236
7	-2.314933	-2.763993	-0.779484
6	-1.341768	-2.313272	0.055877
6	-3.138273	-3.008015	1.263300
6	-3.433896	-3.192084	-0.061936
6	-1.092730	-2.070948	2.508523
1	-0.095428	-1.834210	2.115196
6	-0.935141	-3.209941	3.514915
1	-0.160298	-2.938714	4.246994
1	-0.617819	-4.134908	3.011656
1	-1.858961	-3.412318	4.074318
6	-1.650378	-0.785554	3.114413
1	-1.611634	0.020276	2.369982
1	-1.039402	-0.488680	3.979425
1	-2.687379	-0.899171	3.461923
6	-3.994817	-3.298699	2.450645
1	-4.052703	-2.443833	3.139589
1	-3.632390	-4.165402	3.025593
1	-5.018258	-3.523670	2.123672
6	-4.706339	-3.679796	-0.669079
1	-5.355942	-4.099418	0.110118
1	-4.538963	-4.467306	-1.417347
1	-5.260687	-2.864845	-1.161210
6	-2.110794	-2.844073	-2.238360
1	-1.154882	-2.329396	-2.383643
6	-1.942055	-4.293425	-2.697778
1	-2.882221	-4.862914	-2.640375
1	-1.184191	-4.809049	-2.092419
1	-1.606518	-4.308576	-3.745881
6	-3.170499	-2.080059	-3.032939
1	-4.121587	-2.626616	-3.108251
1	-2.800088	-1.917373	-4.055894
1	-3.364474	-1.094917	-2.588483
6	2.555240	-2.906648	2.208128

1	2.800902	-1.971510	2.735490
1	3.371225	-3.621359	2.404405
1	1.645878	-3.315297	2.669528
6	2.147499	-4.376875	-0.467419
6	3.422530	-5.226637	-0.352447
1	4.248700	-4.808937	-0.947125
1	3.239819	-6.252262	-0.726200
1	3.770405	-5.316387	0.689200
6	1.011419	-5.100523	0.280934
1	0.073412	-4.524060	0.256759
1	1.265413	-5.285230	1.336867
1	0.809478	-6.083923	-0.183817
6	1.752337	-4.259164	-1.948582
1	0.866463	-3.621544	-2.077982
1	1.523529	-5.255154	-2.372636
1	2.553957	-3.818706	-2.557505
6	3.994817	-1.705134	-0.208914
6	3.885172	-0.230946	0.214567
1	3.030785	0.266475	-0.262672
1	4.800397	0.323528	-0.066889
1	3.762373	-0.120802	1.302502
6	5.235152	-2.304981	0.475593
1	6.146235	-1.762486	0.158288
1	5.382661	-3.365340	0.226117
1	5.176448	-2.226030	1.572249
6	4.189906	-1.754065	-1.732939
1	3.301357	-1.393819	-2.273048
1	4.406618	-2.772617	-2.088519
1	5.045142	-1.118534	-2.032221

Table S14

B3LYP-D3(BJ)/def2-SVP

Prod-InIn

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	-1.905129	3.191226	0.437509
49	-0.211478	1.381724	-0.378802
7	2.504236	2.191121	1.292134
7	3.002838	2.256223	-0.805870
6	-0.341749	0.690565	-2.547701
1	-1.432298	0.582216	-2.682956
1	-0.012466	1.361683	-3.366022
6	0.341749	-0.690565	-2.547701
1	1.432298	-0.582216	-2.682956
1	0.012466	-1.361683	-3.366022
14	1.905129	-3.191226	0.437509
49	0.211478	-1.381724	-0.378802
6	1.957726	2.139233	0.049496
6	3.893243	2.331512	1.222235
6	4.208933	2.379615	-0.111526
6	1.673949	2.019058	2.498891
1	0.648181	2.045693	2.107382
6	1.812315	3.181173	3.480466
1	1.011501	3.113945	4.232223
1	1.707465	4.144125	2.959237
1	2.770414	3.172649	4.019077
6	1.874383	0.641668	3.128925
1	1.670211	-0.142333	2.385597
1	1.168810	0.513753	3.963819
1	2.891131	0.503813	3.525502
6	4.809982	2.414150	2.396869
1	4.648288	1.589605	3.106219
1	4.693349	3.358361	2.952117
1	5.853076	2.354918	2.059898
6	5.554466	2.490638	-0.746626
1	6.306126	2.753903	0.009198

1	5.583860	3.266576	-1.525485
1	5.866289	1.541501	-1.210531
6	2.789788	2.306146	-2.265539
1	1.742645	1.999819	-2.377795
6	2.919670	3.735418	-2.791716
1	3.947992	4.119505	-2.703563
1	2.247256	4.411913	-2.244046
1	2.640173	3.764850	-3.855984
6	3.642816	1.294696	-3.031098
1	4.684939	1.622006	-3.155896
1	3.214713	1.158013	-4.034927
1	3.636572	0.316155	-2.531766
6	-2.043317	3.384216	2.336793
1	-2.462516	2.472074	2.789564
1	-2.694728	4.228049	2.620141
1	-1.059694	3.558605	2.797797
6	-1.363945	4.942921	-0.243368
6	-2.454404	6.013345	-0.083906
1	-3.330351	5.803352	-0.716418
1	-2.070510	7.008082	-0.380036
1	-2.804599	6.096102	0.957838
6	-0.125182	5.371701	0.566899
1	0.672204	4.611754	0.519866
1	-0.364522	5.545810	1.627782
1	0.290319	6.314672	0.165071
6	-0.955203	4.849224	-1.723603
1	-0.169879	4.092963	-1.879541
1	-0.564327	5.820974	-2.079717
1	-1.798855	4.575060	-2.373044
6	-3.682811	2.620958	-0.150449
6	-3.845445	1.140114	0.241035
1	-3.089235	0.498381	-0.234649
1	-4.841509	0.766523	-0.062550
1	-3.761041	0.989816	1.328673
6	-4.809982	3.419842	0.525375
1	-5.797940	3.050784	0.189675
1	-4.763528	4.492308	0.288122
1	-4.781178	3.319561	1.621917

6	-3.814724	2.741961	-1.676770
1	-2.991967	2.231698	-2.201958
1	-3.816277	3.792738	-2.003735
1	-4.764619	2.291299	-2.021868
7	-2.504236	-2.191121	1.292134
7	-3.002838	-2.256223	-0.805870
6	-1.957726	-2.139233	0.049496
6	-3.893243	-2.331512	1.222235
6	-4.208933	-2.379615	-0.111526
6	-1.673949	-2.019058	2.498891
1	-0.648181	-2.045693	2.107382
6	-1.812315	-3.181173	3.480466
1	-1.011501	-3.113945	4.232223
1	-1.707465	-4.144125	2.959237
1	-2.770414	-3.172649	4.019077
6	-1.874383	-0.641668	3.128925
1	-1.670211	0.142333	2.385597
1	-1.168810	-0.513753	3.963819
1	-2.891131	-0.503813	3.525502
6	-4.809982	-2.414150	2.396869
1	-4.648288	-1.589605	3.106219
1	-4.693349	-3.358361	2.952117
1	-5.853076	-2.354918	2.059898
6	-5.554466	-2.490638	-0.746626
1	-6.306126	-2.753903	0.009198
1	-5.583860	-3.266576	-1.525485
1	-5.866289	-1.541501	-1.210531
6	-2.789788	-2.306146	-2.265539
1	-1.742645	-1.999819	-2.377795
6	-2.919670	-3.735418	-2.791716
1	-3.947992	-4.119505	-2.703563
1	-2.247256	-4.411913	-2.244046
1	-2.640173	-3.764850	-3.855984
6	-3.642816	-1.294696	-3.031098
1	-4.684939	-1.622006	-3.155896
1	-3.214713	-1.158013	-4.034927
1	-3.636572	-0.316155	-2.531766
6	2.043317	-3.384216	2.336793

1	2.462516	-2.472074	2.789564
1	2.694728	-4.228049	2.620141
1	1.059694	-3.558605	2.797797
6	1.363945	-4.942921	-0.243368
6	2.454404	-6.013345	-0.083906
1	3.330351	-5.803352	-0.716418
1	2.070510	-7.008082	-0.380036
1	2.804599	-6.096102	0.957838
6	0.125182	-5.371701	0.566899
1	-0.672204	-4.611754	0.519866
1	0.364522	-5.545810	1.627782
1	-0.290319	-6.314672	0.165071
6	0.955203	-4.849224	-1.723603
1	0.169879	-4.092963	-1.879541
1	0.564327	-5.820974	-2.079717
1	1.798855	-4.575060	-2.373044
6	3.682811	-2.620958	-0.150449
6	3.845445	-1.140114	0.241035
1	3.089235	-0.498381	-0.234649
1	4.841509	-0.766523	-0.062550
1	3.761041	-0.989816	1.328673
6	4.809982	-3.419842	0.525375
1	5.797940	-3.050784	0.189675
1	4.763528	-4.492308	0.288122
1	4.781178	-3.319561	1.621917
6	3.814724	-2.741961	-1.676770
1	2.991967	-2.231698	-2.201958
1	3.816277	-3.792738	-2.003735
1	4.764619	-2.291299	-2.021868

Table S15

B3LYP-D3(BJ)/def2-SVP

Prod-TlTl

Atomic Number	Coordinates (Angstroms) X	Y	Z
14	1.492859	3.490324	0.548419
81	0.917185	1.102258	-0.407806
7	3.220726	-0.773793	1.309336
7	3.572846	-1.148495	-0.781667
6	0.337170	0.680005	-2.666905
1	-0.373693	1.494653	-2.875656
1	1.167425	0.788199	-3.388203
6	-0.337170	-0.680005	-2.666905
1	0.373693	-1.494653	-2.875656
1	-1.167425	-0.788199	-3.388203
14	-1.492859	-3.490324	0.548419
81	-0.917185	-1.102258	-0.407806
6	2.903702	-0.329532	0.065630
6	4.087557	-1.870418	1.248199
6	4.318002	-2.102848	-0.083097
6	2.605138	-0.178949	2.508196
1	2.064166	0.689325	2.110961
6	3.637972	0.343027	3.505351
1	3.130677	0.960140	4.262310
1	4.383520	0.972892	2.997967
1	4.161181	-0.464605	4.036557
6	1.561823	-1.109426	3.124511
1	0.808931	-1.376556	2.369622
1	1.050990	-0.594912	3.952050
1	2.006399	-2.031204	3.527205
6	4.631406	-2.609748	2.425338
1	3.836118	-2.960936	3.099547
1	5.324794	-1.995599	3.021552
1	5.183317	-3.495557	2.084808
6	5.147501	-3.171547	-0.712402
1	5.781915	-3.650335	0.045348

1	5.810660	-2.774856	-1.494935
1	4.525417	-3.957325	-1.169930
6	3.506406	-0.938251	-2.239060
1	2.663728	-0.246247	-2.352298
6	4.763650	-0.235911	-2.751501
1	5.662420	-0.863608	-2.644204
1	4.929200	0.703522	-2.203244
1	4.647488	0.006158	-3.819153
6	3.159000	-2.209914	-3.013160
1	4.018389	-2.884459	-3.133609
1	2.811775	-1.930871	-4.018765
1	2.344547	-2.759208	-2.520202
6	1.575392	3.605289	2.454745
1	0.591042	3.393060	2.900830
1	1.885041	4.610314	2.788621
1	2.290777	2.883252	2.874684
6	3.239400	4.053776	-0.115369
6	3.506406	5.549459	0.114876
1	2.849632	6.182110	-0.501847
1	4.548916	5.804394	-0.154250
1	3.360948	5.840393	1.168049
6	4.292756	3.231419	0.653135
1	4.104754	2.149015	0.559468
1	4.313399	3.482426	1.725324
1	5.302877	3.431304	0.250141
6	3.389334	3.733672	-1.613048
1	3.238748	2.661142	-1.814228
1	4.403220	4.002699	-1.963846
1	2.668779	4.285934	-2.234013
6	-0.004724	4.630521	0.022474
6	-1.303941	3.922597	0.453194
1	-1.422293	2.938157	-0.023602
1	-2.183559	4.533549	0.177106
1	-1.348580	3.764417	1.541906
6	0.041680	6.006379	0.708630
1	-0.843817	6.607643	0.427536
1	0.932868	6.584732	0.426017
1	0.037799	5.914846	1.806242

6	-0.036336	4.816240	-1.502570
1	-0.021300	3.850146	-2.032475
1	0.820587	5.405935	-1.862004
1	-0.954071	5.352370	-1.809611
7	-3.220726	0.773793	1.309336
7	-3.572846	1.148495	-0.781667
6	-2.903702	0.329532	0.065630
6	-4.087557	1.870418	1.248199
6	-4.318002	2.102848	-0.083097
6	-2.605138	0.178949	2.508196
1	-2.064166	-0.689325	2.110961
6	-3.637972	-0.343027	3.505351
1	-3.130677	-0.960140	4.262310
1	-4.383520	-0.972892	2.997967
1	-4.161181	0.464605	4.036557
6	-1.561823	1.109426	3.124511
1	-0.808931	1.376556	2.369622
1	-1.050990	0.594912	3.952050
1	-2.006399	2.031204	3.527205
6	-4.631406	2.609748	2.425338
1	-3.836118	2.960936	3.099547
1	-5.324794	1.995599	3.021552
1	-5.183317	3.495557	2.084808
6	-5.147501	3.171547	-0.712402
1	-5.781915	3.650335	0.045348
1	-5.810660	2.774856	-1.494935
1	-4.525417	3.957325	-1.169930
6	-3.506406	0.938251	-2.239060
1	-2.663728	0.246247	-2.352298
6	-4.763650	0.235911	-2.751501
1	-5.662420	0.863608	-2.644204
1	-4.929200	-0.703522	-2.203244
1	-4.647488	-0.006158	-3.819153
6	-3.159000	2.209914	-3.013160
1	-4.018389	2.884459	-3.133609
1	-2.811775	1.930871	-4.018765
1	-2.344547	2.759208	-2.520202
6	-1.575392	-3.605289	2.454745

1	-0.591042	-3.393060	2.900830
1	-1.885041	-4.610314	2.788621
1	-2.290777	-2.883252	2.874684
6	-3.239400	-4.053776	-0.115369
6	-3.506406	-5.549459	0.114876
1	-2.849632	-6.182110	-0.501847
1	-4.548916	-5.804394	-0.154250
1	-3.360948	-5.840393	1.168049
6	-4.292756	-3.231419	0.653135
1	-4.104754	-2.149015	0.559468
1	-4.313399	-3.482426	1.725324
1	-5.302877	-3.431304	0.250141
6	-3.389334	-3.733672	-1.613048
1	-3.238748	-2.661142	-1.814228
1	-4.403220	-4.002699	-1.963846
1	-2.668779	-4.285934	-2.234013
6	0.004724	-4.630521	0.022474
6	1.303941	-3.922597	0.453194
1	1.422293	-2.938157	-0.023602
1	2.183559	-4.533549	0.177106
1	1.348580	-3.764417	1.541906
6	-0.041680	-6.006379	0.708630
1	0.843817	-6.607643	0.427536
1	-0.932868	-6.584732	0.426017
1	-0.037799	-5.914846	1.806242
6	0.036336	-4.816240	-1.502570
1	0.021300	-3.850146	-2.032475
1	-0.820587	-5.405935	-1.862004
1	0.954071	-5.352370	-1.809611