Electronic Supplementary Information (ESI)

Phosphine and Solvent effects on Oxidative Addition of CH_3Br to PdL and PdL_2 Complexes.

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Summary

2.- Tables.

Table S1 Relative free energies of the concerted and S_N2 transition states and products respect to CH_3Br and Palladium bis-phosphine, energies in kcal/mol.

		Gas phase	Gas phase	Gas phase	Gas phase	THF	THF	THF	THF	DMF	DMF	DMF	DMF
		conc*cis*	conc*trans*	S_N2*cis*	S_N2*trans*	conc*cis*	conc*trans*	S_N2*cis*	S_N2*trans*	conc*cis*	conc*trans*	S_N2*cis*	$S_N2$trans
TS	**PF_3**	23.8	23.1	48.4	46.9	26.1	25.9	--	27.4	27.3	27.2	--	24.5
Product	**PF_3**	-2.8	-2.9	--	--	-2.5	-2.7	--	--	-1.6	-2.1	--	22.8
TS	**PH_3**	26.4	26.0	35.3	26.6	26.4	24.9	--	10.6	26.6	25.7	--	9.5
Product	**PH_3**	-11.0	-15.6	--	--	-17.4	-21.5	--	2.8	-19.6	-22.4	--	-2.8
TS	**$P(CH_3)_3$**	--	26.2	25.2	12.3	--	27.0	--	6.4	--	28.2	--	6.4
Product	**$P(CH_3)_3$**	-23.1	-32.3	--	12.0	-27.6	-33.9	--	-9.6	-27.9	-33.3	--	-16.6
TS	**PPh_3**	19.4	21.1	--	8.9	21.0	22.1	--	2.8	21.9	22.7	--	2.3
Product	**PPh_3**	-21.9	-26.4	--	8.4	-27.8	-28.1	--	-13.4	-28.3	-30.7	--	-17.9

Table S2 Relative free energies of the concerted and S_N2 transition states and products respect to CH_3Br in Palladium mono-phosphine, energies in kcal/mol.

		Gas phase	Gas phase	Gas phase	Gas phase	THF	THF	THF	THF	DMF	DMF	DMF	DMF
		conc1	conc2	S_N21	S_N22	conc1	conc2	S_N21	S_N22	conc1	conc2	S_N21	S_N22
TS	**PF_3**	5.1	8.2	37.8	48.3	14.3	17.6	18.0	34.6	17.3	19.4	16.2	--
Product	**PF_3**	-16.4	-3.3	--	--	-13.2	-0.4	17.4	--	-12.6	-1.5	11.3	--
TS	**PH_3**	4.8	7.0	29.8	39.6	7.8	10.2	9.8	18.4	10.0	10.9	7.6	15.8
Product	**PH_3**	-22.8	-10.1	--	--	-27.1	-13.7	-0.8	15.8	-29.6	-14.9	-7.2	13.5
TS	**$P(CH_3)_3$**	6.3	7.7	22.9	38.2	7.6	10.5	7.3	17.8	8.8	11.1	6.1	15.9
Product	**$P(CH_3)_3$**	-27.1	-13.2	--	--	-34.7	-15.7	-9.4	19.0	-36.3	-17.1	-17.6	11.3
TS	**PPh_3**	3.9	7.0	17.7	35.9	6.6	9.5	7.1	18.9	9.5	12.1	4.4	15.8
Product	**PPh_3**	-30.4	-14.2	--	--	-34.3	-14.2	-7.0	18.4	-34.6	-15.1	-14.8	11.6

Table S3 Dissociation energies of $Pd(PR_3)_2$ to $Pd(PR_3)$ and PR_3 in gas phase, THF, and DMF are presented for the studied phosphines. The dissociation energies decrease with the dielectric constant and encrease as $PF_3 < PH_3 < PMe_3 < PPh_3$. This is due to the donor properties of the phosphines which follow $PF_3 < PH_3 < PPh_3 < PMe_3$, and to the dispersion energies, which make the dissoaciation energy in $Pd(PPh_3)_2$ larger than in $Pd(PMe_3)_2$. energies in kcal/mol.

	Gas phase	THF	DMF
PF_3	19.3	12.1	11.4
PH_3	19.3	15.6	14.7
PMe_3	24.9	21.6	22.3
PPh_3	32.7	28.2	27.4

2.- Coordinates (in Å) and Energies (in hartree) of the located species.

2.1 Bis-phosphine Palladium catalyst

2.1.1 Species Optimized in gas phase

CH_3Br

ΔE_{gas} -2611.32581405
ΔE_{gas} (ZPE) -2611.288609
ΔG_{gas} -2611.312491

6	0.000000	0.000000	-1.543092
35	0.000000	0.000000	0.425114
1	0.000000	1.036549	-1.873486
1	0.897678	-0.518275	-1.873486
1	-0.897678	-0.518275	-1.873486

2.1.1.1 PF_3

$Pd(PF_3)_2$

ΔE_{gas} -1409.95465808
ΔE_{gas} (ZPE) -1409.935430
ΔG_{gas} -1409.979625

46	0.000155	-0.453993	-0.000997
15	2.184055	0.101928	-0.001604
15	-2.184099	0.102471	0.001277
9	-3.165114	-0.408916	1.154835
9	-3.110949	-0.260785	-1.248975
9	-2.539314	1.655137	0.090472
9	3.347129	-0.970269	-0.243799
9	2.790239	0.775483	1.312854
9	2.677287	1.189091	-1.059745

Adduct Conccis

ΔE_{gas} -4021.29555266
ΔE_{gas} (ZPE) -4021.238424
ΔG_{gas} -4021.291234

15	-0.891239	2.018813	-0.005460
46	0.132838	0.024367	0.014223
15	2.351906	-0.324845	0.000570
35	-1.405670	-2.160128	-0.017911
6	-3.293641	-1.558254	0.037154
1	-3.401473	-0.772696	-0.706296
1	-3.902503	-2.428496	-0.198346
1	-3.483122	-1.192824	1.043436
9	3.050819	-1.124089	-1.204463
9	3.336495	0.940529	-0.022518
9	3.068244	-1.094096	1.214896
9	-0.910900	2.891927	1.339766
9	-2.454040	2.206283	-0.373968
9	-0.343189	3.159182	-0.988794

TS Conccis

ΔE_{gas} -4021.24925242
ΔE_{gas} (ZPE) -4021.193940
ΔG_{gas} -4021.244412

15	1.537974	-1.578062	0.022009
46	-0.036496	0.148275	0.136144
15	-2.238289	-0.415740	-0.115041
35	1.154664	2.291936	-0.402636
6	-0.262961	1.987390	1.571513
1	0.533216	2.532563	2.058593
1	-1.100170	2.595334	1.250645
1	-0.530362	1.079021	2.126170
9	-2.864908	-0.283176	-1.580149
9	-2.753303	-1.901385	0.193186
9	-3.393607	0.358263	0.691309
9	1.177313	-2.947375	-0.726609
9	2.006284	-2.213853	1.416941
9	2.988820	-1.374990	-0.621276

Product Conccis

ΔE_{gas} -4021.29237369
ΔE_{gas} (ZPE) -4021.234711
ΔG_{gas} -4021.282091

46	0.116388	-0.476065	-0.000088
15	-0.985217	1.635769	0.000014
35	-2.203821	-1.364531	0.000022
6	0.763563	-2.479396	-0.000249
1	0.312201	-2.894380	0.900594
1	0.311610	-2.894395	-0.900784
1	1.843427	-2.632353	-0.000609
15	2.274878	0.035054	0.000061
9	3.172432	-0.476274	1.203343
9	3.172518	-0.475667	-1.203419
9	2.721168	1.559087	0.000469
9	-0.130143	2.985660	0.000003
9	-1.946562	1.975436	-1.211219
9	-1.946482	1.975400	1.211321

Adduct Conctrans

ΔE_{gas} -4021.29555266
ΔE_{gas} (ZPE) -4021.238426
ΔG_{gas} -4021.291274

15	0.893239	2.017592	-0.005637
46	-0.133277	0.024259	0.013786
15	-2.352568	-0.322928	0.000709
35	1.404231	-2.160737	-0.018196
6	3.292300	-1.559132	0.038436
1	3.480945	-1.193619	1.044847
1	3.901212	-2.429494	-0.196436
1	3.400893	-0.773698	-0.705021
9	-3.052571	-1.122098	-1.203754
9	-3.335991	0.943366	-0.022748
9	-3.069307	-1.090960	1.215576
9	2.455667	2.203178	-0.376642
9	0.345197	3.160216	-0.986326
9	0.916535	2.888693	1.340851

TS Conctrans

ΔE_{gas} -4021.24908465
ΔE_{gas} (ZPE) -4021.193863
ΔG_{gas} -4021.245257

15	2.082384	-0.993986	-0.059753
46	0.000032	0.020753	-0.001935
15	-2.082309	-0.994130	-0.059902
35	-0.000169	2.495722	-0.349705
6	0.000251	1.381850	1.876036
1	0.914047	1.916617	2.099793
1	-0.912774	1.917788	2.100121
1	-0.000451	0.343646	2.228460
9	-3.158593	-0.546238	1.043757
9	-2.275891	-2.575864	0.115961
9	-3.002199	-0.819842	-1.356903
9	3.162579	-0.539440	1.037340
9	2.276587	-2.574615	0.125222
9	2.997626	-0.827592	-1.361054

Product Conctrans

ΔE_{gas} -4021.29147095
ΔE_{gas} (ZPE) -4021.233739
ΔG_{gas} -4021.281371

46	0.002663	-0.450347	0.000002
15	-2.271158	-0.377810	0.000003
15	2.278230	-0.346853	0.000019
6	0.065568	-2.546082	-0.000134
1	0.602557	-2.865539	-0.896851
1	0.604667	-2.865918	0.895160
1	-0.936660	-2.971760	0.000977
35	-0.029473	2.086204	-0.000039
9	-3.123249	-1.721194	-0.000052
9	-2.977441	0.347507	-1.211179
9	-2.977273	0.347329	1.211408
9	2.977550	0.385463	-1.211184
9	2.977511	0.385606	1.211167
9	3.138347	-1.683771	0.000114

Adduct S_N2cis

ΔE_{gas} -4021.29555238
ΔE_{gas} (ZPE) -4021.238433
ΔG_{gas} -4021.291321

6	3.290154	-1.559400	0.045090
1	3.899782	-2.426936	-0.198200
1	3.399201	-0.765999	-0.689768
1	3.477209	-1.204676	1.055646
35	1.402479	-2.161450	-0.020066
15	-2.354283	-0.319462	0.001296
46	-0.134433	0.024085	0.013074
15	0.896739	2.014964	-0.005840
9	0.919315	2.887882	1.339414
9	0.354743	3.157842	-0.989656
9	2.460862	2.195254	-0.372856
9	-3.056651	-1.116447	-1.203241
9	-3.336033	0.948145	-0.019777
9	-3.070769	-1.087750	1.216213

TS S_N2cis

ΔE_{gas} -4021.20624767
ΔE_{gas} (ZPE) -4021.152609
ΔG_{gas} -4021.203272

6	-0.911989	-1.921879	0.000193
1	-0.817309	-2.521493	0.907236
1	-0.817878	-2.520981	-0.907249
1	-1.799386	-1.205850	0.000642
35	-3.738399	-0.564521	-0.000011
15	2.065648	-1.341147	-0.000016
46	0.187445	-0.152952	-0.000073
15	0.553397	2.178571	-0.000003

9	0.002064	3.039982	-1.212410
9	2.055699	2.702807	0.000168
9	0.001857	3.039822	1.212425
9	2.347048	-2.330739	-1.208406
9	2.347153	-2.330343	1.208675
9	3.450882	-0.564613	-0.000203

Product S_N2cis

ΔE_{gas} -4021.29237369
ΔE_{gas} (ZPE) -4021.234711
ΔG_{gas} -4021.282091

46	0.116388	-0.476065	-0.000088
15	-0.985217	1.635769	0.000014
35	-2.203821	-1.364531	0.000022
6	0.763563	-2.479396	-0.000249
1	0.312201	-2.894380	0.900594
1	0.311610	-2.894395	-0.900784
1	1.843427	-2.632353	-0.000609
15	2.274878	0.035054	0.000061
9	3.172432	-0.476274	1.203343
9	3.172518	-0.475667	-1.203419
9	2.721168	1.559087	0.000469
9	-0.130143	2.985660	0.000003
9	-1.946562	1.975436	-1.211219
9	-1.946482	1.975400	1.211321

Adduct $S_N2trans$

ΔE_{gas} -4021.29547997
ΔE_{gas} (ZPE) -4021.238349
ΔG_{gas} -4021.290838

6	3.220841	-1.706774	0.000483
1	3.399827	-1.125119	-0.900471
1	3.399614	-1.126573	0.902421
1	3.784637	-2.637241	-0.000194
35	1.303641	-2.208251	-0.000121
15	-2.362641	-0.245543	0.000100
9	-3.089171	-1.012303	-1.209920
9	-3.089213	-1.013438	1.209388
9	-3.315709	1.043539	0.000718
46	-0.132993	0.045097	-0.000115
15	0.971168	1.994252	-0.000047
9	1.969504	2.364013	-1.207365
9	0.162467	3.377633	-0.000755
9	1.968037	2.364251	1.208387

TS $S_N2trans$

ΔE_{gas} -4021.21095901
ΔE_{gas} (ZPE) -4021.155388
ΔG_{gas} -4021.204436

6	0.145123	-1.623793	0.010575
1	0.637284	-1.385769	0.947717
1	0.636796	-1.384128	-0.926789
1	-0.440317	-2.542581	0.007948
35	2.957515	-1.592640	-0.002016
15	1.466339	1.383919	0.001824
9	2.442580	1.522479	1.238877
9	2.450724	1.530377	-1.227827
9	0.944518	2.908404	0.004777
46	-0.791539	0.312610	-0.006287
15	-2.940866	-0.290372	0.000834
9	-3.622460	-0.675472	1.382680
9	-4.034569	0.729773	-0.535610
9	-3.368441	-1.569521	-0.837615

Product $S_N2trans$

ΔE_{gas} -4021.29147095
ΔE_{gas} (ZPE) -4021.233739
ΔG_{gas} -4021.281371

46	0.002663	-0.450347	0.000002
15	-2.271158	-0.377810	0.000003
15	2.278230	-0.346853	0.000019
6	0.065568	-2.546082	-0.000134
1	0.602557	-2.865539	-0.896851
1	0.604667	-2.865918	0.895160
1	-0.936660	-2.971760	0.000977
35	-0.029473	2.086204	-0.000039
9	-3.123249	-1.721194	-0.000052
9	-2.977441	0.347507	-1.211179
9	-2.977273	0.347329	1.211408
9	2.977550	0.385463	-1.211184
9	2.977511	0.385606	1.211167
9	3.138347	-1.683771	0.000114

2.1.1.2 PH_3

$Pd(PH_3)_2$

ΔE_{gas} -814.278506515
ΔE_{gas} (ZPE) -814.224859
ΔG_{gas} -814.256947

46	-0.000001	-0.003373	-0.000488
15	-2.289307	0.003985	0.000575
1	-3.012921	-0.383507	1.156205
1	-3.009121	1.201175	-0.239539
1	-3.015017	-0.799855	-0.914062
15	2.289311	0.003978	0.000561
1	3.009651	0.811766	0.915809
1	3.015575	-1.189325	0.241356
1	3.011842	0.395447	-1.154370

Adduct Conccis

ΔE_{gas} -3425.60255736
ΔE_{gas} (ZPE) -3425.511626
ΔG_{gas} -3425.559599

15	1.945651	-1.907677	0.000269
46	0.779656	0.074101	-0.000199
15	1.362716	2.291513	-0.000414
35	-1.959793	-0.582442	-0.000614
1	2.892340	-2.147342	-1.029507
1	2.834717	-2.177527	1.073045
1	1.394879	-3.220750	-0.033834
1	0.484330	3.414590	-0.027241
1	2.153964	2.790878	1.067122
1	2.203390	2.779664	-1.034769
6	-3.142082	0.999710	0.001862
1	-4.169691	0.641327	-0.001917
1	-2.921427	1.567010	0.903376
1	-2.916939	1.573159	-0.894641

TS Conccis

ΔE_{gas} -3425.56601535
ΔE_{gas} (ZPE) -3425.476846
ΔG_{gas} -3425.519391

15	1.200321	2.300529	-0.000664
46	0.499638	0.031402	0.101954
15	1.890691	-1.826837	-0.333054
35	-2.021199	-0.061621	-0.381986
1	2.379127	2.728102	-0.666529
1	0.360703	3.299280	-0.559326
1	1.473210	3.003718	1.202195
1	1.636976	-3.139793	0.153266
1	2.016228	-2.209561	-1.692766
1	3.282815	-1.862900	-0.054604
6	-1.084648	-0.875715	1.610625
1	-1.896052	-0.392565	2.139980
1	-1.240679	-1.933978	1.436413
1	-0.110989	-0.631128	2.063043

Product Conccis

ΔE_{gas} -3425.62815085
ΔE_{gas} (ZPE) -3425.535613
ΔG_{gas} -3425.574884

15	0.076314	2.247228	0.000004
46	-0.420450	-0.120692	0.000042
15	-2.687294	-0.163353	-0.000043
35	2.075322	-0.367435	-0.000015
1	-0.882619	3.295947	-0.001145
1	0.869612	2.706866	1.070924
1	0.871078	2.705478	-1.070373
1	-3.326873	-0.828630	-1.068930
1	-3.326696	-0.828573	1.068988
1	-3.461333	1.021267	-0.000049
6	-0.548227	-2.207114	-0.000036
1	-0.012804	-2.525120	0.896490
1	-1.560150	-2.625458	-0.000634
1	-0.011717	-2.525156	-0.895877

Adduct Conctrans

ΔE_{gas} -3425.60632328
ΔE_{gas} (ZPE) -3425.514779
ΔG_{gas} -3425.563341

15	-1.718046	-2.290755	-0.061254
46	-1.657575	0.000008	-0.015347
15	-1.717630	2.290869	-0.061474
35	3.434844	-0.000247	-0.239950
6	2.080065	0.000641	1.191719
1	2.234731	-0.896339	1.788134
1	2.234692	0.898398	1.786974
1	1.095515	0.000307	0.720769
1	-1.183413	3.069021	0.996083
1	-2.964813	2.958803	-0.133283
1	-1.091057	3.003153	-1.113610
1	-1.095357	-3.003240	-1.115556
1	-1.180778	-3.069434	0.994369
1	-2.965856	-2.957954	-0.129045

TS Conctrans

ΔE_{gas} -3425.56586041
ΔE_{gas} (ZPE) -3425.476883
ΔG_{gas} -3425.520214

15	-1.495724	-2.153552	-0.165418
46	-0.525863	0.000006	0.067608
15	-1.495622	2.153623	-0.165367
35	1.998111	-0.000012	-0.383275
6	1.078305	-0.000127	1.791708
1	1.606952	-0.909310	2.050435
1	1.607171	0.908889	2.050578
1	0.032842	-0.000010	2.137314
1	-0.974426	3.292510	0.506167
1	-2.856300	2.470182	0.090884
1	-1.464478	2.735921	-1.458022
1	-1.464472	-2.735878	-1.458058
1	-0.974673	-3.292456	0.506197
1	-2.856449	-2.470024	0.090689

Product Conctrans

ΔE_{gas} -3425.63470888
ΔE_{gas} (ZPE) -3425.542062
ΔG_{gas} -3425.581584

46	0.582536	0.058296	0.000068
15	0.264890	2.348847	0.000007
1	1.345158	3.263131	0.000101
1	-0.481139	2.871226	-1.074873
1	-0.481299	2.871204	1.074794
15	0.713868	-2.254989	-0.000084
1	0.087242	-2.916636	1.074388
1	0.087948	-2.916457	-1.075074
1	1.956393	-2.932473	0.000248
6	2.657162	0.214529	0.000529
1	3.046424	-0.283820	0.894911
1	3.046836	-0.283893	-0.893630
1	2.994812	1.253462	0.000560
35	-1.972096	-0.180069	-0.000188

Adduct S_N2cis

ΔE_{gas} -3425.60716512
ΔE_{gas} (ZPE) -3425.515563
ΔG_{gas} -3425.563113

6	1.825878	-1.700202	-0.005782
1	1.974366	-2.289483	-0.908400
1	1.976017	-2.300323	0.889364
1	0.850439	-1.210107	-0.002150
35	3.196758	-0.281571	0.001516
15	-2.990089	-1.467845	0.001368
1	-2.982589	-2.430242	-1.039705
1	-3.017093	-2.398501	1.070565
1	-4.385062	-1.220733	-0.025331
46	-1.531479	0.292250	-0.000126
15	-0.176151	2.150877	-0.000942
1	0.724315	2.398067	1.062263
1	0.740002	2.386405	-1.053310
1	-0.780542	3.432135	-0.012245

TS S_N2cis

ΔE_{gas} -3425.54838062
ΔE_{gas} (ZPE) -3425.459341
ΔG_{gas} -3425.503572

6	-0.503164	-1.483959	-0.005416
1	-0.527521	-2.101827	0.895337
1	-0.527070	-2.091400	-0.913209
1	-1.297824	-0.677357	-0.000464
35	-3.303560	0.067497	0.001231
15	2.452633	-1.652501	0.002933
1	2.491753	-2.542729	1.097344
1	2.450233	-2.597430	-1.045209
1	3.819302	-1.296399	-0.032812
46	0.914154	0.002337	-0.001467
15	1.816217	2.252816	0.000489
1	1.434038	3.129810	-1.039647
1	1.510059	3.099522	1.089716
1	3.206767	2.506940	-0.045483

Product S_N2cis

ΔE_{gas} -3425.62815085
ΔE_{gas} (ZPE) -3425.535613
ΔG_{gas} -3425.574884

15	0.076314	2.247228	0.000004
46	-0.420450	-0.120692	0.000042
15	-2.687294	-0.163353	-0.000043
35	2.075322	-0.367435	-0.000015
1	-0.882619	3.295947	-0.001145
1	0.869612	2.706866	1.070924
1	0.871078	2.705478	-1.070373
1	-3.326873	-0.828630	-1.068930
1	-3.326696	-0.828573	1.068988
1	-3.461333	1.021267	-0.000049
6	-0.548227	-2.207114	-0.000036
1	-0.012804	-2.525120	0.896490
1	-1.560150	-2.625458	-0.000634
1	-0.011717	-2.525156	-0.895877

Adduct $S_N2trans$

ΔE_{gas} -3425.60716512
ΔE_{gas} (ZPE) -3425.515563
ΔG_{gas} -3425.563113

6	1.825878	-1.700202	-0.005782
1	1.974366	-2.289483	-0.908400
1	1.976017	-2.300323	0.889364
1	0.850439	-1.210107	-0.002150
35	3.196758	-0.281571	0.001516
15	-2.990089	-1.467845	0.001368
1	-2.982589	-2.430242	-1.039705
1	-3.017093	-2.398501	1.070565
1	-4.385062	-1.220733	-0.025331
46	-1.531479	0.292250	-0.000126
15	-0.176151	2.150877	-0.000942
1	0.724315	2.398067	1.062263
1	0.740002	2.386405	-1.053310
1	-0.780542	3.432135	-0.012245

TS $S_N2trans$

ΔE_{gas} -3425.56462878
ΔE_{gas} (ZPE) -3425.473358
ΔG_{gas} -3425.514048

6	0.305267	-0.926494	0.002049
1	0.759943	-0.572532	0.921508
1	0.758502	-0.569687	-0.917207
1	0.082859	-1.993356	-0.000730
35	3.207091	-0.563847	-0.000247
15	0.103083	2.175665	0.003424
46	-1.420833	0.332967	-0.003042
15	-2.903819	-1.436240	0.002677
1	0.120987	3.097175	-1.065333
1	0.120545	3.088341	1.079749
1	1.454359	1.741444	0.002158
1	-4.253478	-1.227851	-0.360987
1	-2.632673	-2.546098	-0.826788
1	-3.121474	-2.131717	1.212422

Product $S_N2$trans

ΔE_{gas} -3425.63470888
ΔE_{gas} (ZPE) -3425.542062
ΔG_{gas} -3425.581584

46	0.582536	0.058296	0.000068
15	0.264890	2.348847	0.000007
1	1.345158	3.263131	0.000101
1	-0.481139	2.871226	-1.074873
1	-0.481299	2.871204	1.074794
15	0.713868	-2.254989	-0.000084
1	0.087242	-2.916636	1.074388
1	0.087948	-2.916457	-1.075074
1	1.956393	-2.932473	0.000248
6	2.657162	0.214529	0.000529
1	3.046424	-0.283820	0.894911
1	3.046836	-0.283893	-0.893630
1	2.994812	1.253462	0.000560
35	-1.972096	-0.180069	-0.000188

2.1.1.3 $P(CH_3)_3$

$Pd(P(CH_3)_3)_2$

ΔE_{gas} -1050.22988478
ΔE_{gas} (ZPE) -1050.001593
ΔG_{gas} -1050.045670

46	-0.000109	-0.003819	-0.004828
15	2.306287	0.000122	0.001856
15	-2.306006	0.000461	-0.000097
6	-3.156518	0.342552	-1.613907
1	-2.841520	-0.397870	-2.354940
1	-4.248001	0.310236	-1.513562
1	-2.858161	1.329324	-1.979830
6	-3.148882	1.231622	1.103666
1	-2.837314	2.242487	0.825040
1	-4.240734	1.159099	1.034095
1	-2.842251	1.061221	2.139796
6	-3.155255	-1.567431	0.514487
1	-2.847554	-1.830831	1.530613
1	-4.246825	-1.468375	0.482664
1	-2.848685	-2.381259	-0.149044
6	3.149065	-0.347125	1.618490
1	4.240880	-0.306589	1.525082
1	2.824351	0.386092	2.362501
1	2.855320	-1.338362	1.975991
6	3.163354	-1.218769	-1.104529
1	4.254289	-1.140701	-1.027491
1	2.855726	-2.233244	-0.834605
1	2.862419	-1.043425	-2.141524
6	3.148458	1.576695	-0.497426
1	2.830240	2.384515	0.168029
1	4.240465	1.485906	-0.457355
1	2.846793	1.843462	-1.514481

Product Conccis

ΔE_{gas} -3661.58886101
ΔE_{gas} (ZPE) -3661.321306
ΔG_{gas} -3661.371234

6	-0.780881	-2.465129	0.070563
1	-0.455881	-2.906822	-0.875259
1	-1.851948	-2.637033	0.207862
1	-0.231838	-2.925909	0.894116
35	2.212681	-1.471422	-0.026277
15	-2.348984	0.048643	-0.011209
46	-0.121698	-0.473652	0.021720
15	1.039907	1.677718	0.005976
6	-3.281417	-0.704277	-1.417645
1	-3.134172	-1.785620	-1.432732
1	-4.351363	-0.483339	-1.338039
1	-2.900782	-0.295723	-2.358168
6	-3.299663	-0.491294	1.478789
1	-4.367196	-0.276208	1.359103
1	-3.162296	-1.561236	1.646799
1	-2.922973	0.041866	2.356400
6	-2.901846	1.809630	-0.147901
1	-2.540646	2.388502	0.705183
1	-2.507793	2.257556	-1.063521
1	-3.995848	1.861026	-0.172052
6	2.205438	1.845193	1.429496
1	1.636308	1.890315	2.363113
1	2.848137	0.962966	1.457067
1	2.813021	2.751913	1.333935
6	2.134581	1.882913	-1.467628
1	1.521678	1.951433	-2.371628
1	2.748826	2.785879	-1.379597
1	2.773650	1.000928	-1.547468
6	0.212996	3.342166	0.055950
1	-0.438398	3.477381	-0.811413
1	-0.390899	3.440814	0.962477
1	0.965593	4.138461	0.053111

Adduct Conctrans

ΔE_{gas} -3661.55862153
ΔE_{gas} (ZPE) -3661.292559
ΔG_{gas} -3661.352365

15	1.788044	-1.657771	-0.000106
46	-0.365712	-0.819296	0.000488
15	-2.580285	-0.161551	-0.000032
35	0.986822	2.263052	0.001396
6	1.803671	4.076172	-0.002769
1	2.754407	4.011736	-0.528782
1	1.117806	4.748019	-0.515571
1	1.947936	4.378715	1.032777
6	-3.594961	-0.682923	1.464401
1	-3.162514	-0.257849	2.374717
1	-4.637390	-0.354160	1.372694
1	-3.567857	-1.772439	1.556350
6	-3.625999	-0.797516	-1.395724
1	-4.665980	-0.460065	-1.308062
1	-3.213299	-0.447687	-2.346345
1	-3.601119	-1.890938	-1.400675
6	-2.975183	1.649477	-0.070018
1	-4.057864	1.824109	-0.064587
1	-2.521462	2.155139	0.786769
1	-2.543192	2.081238	-0.977074
6	2.876375	-1.202304	1.431172
1	3.876309	-1.642642	1.336503
1	2.962570	-0.113421	1.482516
1	2.417135	-1.549481	2.361288
6	1.956300	-3.505999	-0.001131
1	1.459077	-3.914920	-0.885384
1	3.007846	-3.818157	-0.002013
1	1.460298	-3.915895	0.883356
6	2.874243	-1.201535	-1.432829
1	3.874990	-1.640190	-1.338898
1	2.414569	-1.550137	-2.362196
1	2.958668	-0.112569	-1.485202

TS Conctrans

ΔE_{gas} -3661.51524753
ΔE_{gas} (ZPE) -3661.250857
ΔG_{gas} -3661.304955

15	-2.226629	-0.937513	0.038119
46	0.000449	-0.139359	-0.181380
15	2.228229	-0.935092	0.038432
35	-0.002705	2.418097	0.412162
6	0.000230	1.615229	-1.788789
1	-0.907132	2.154812	-2.031774
1	0.907473	2.155752	-2.030129
1	0.001039	0.582405	-2.172424
6	2.879010	-0.818294	1.773668
1	3.925525	-1.139795	1.837571
1	2.795881	0.216190	2.118868
1	2.270365	-1.442926	2.433990
6	3.570797	-0.034536	-0.881450
1	3.531243	1.029248	-0.628362
1	4.566243	-0.423202	-0.634912
1	3.410737	-0.134257	-1.959791
6	2.675071	-2.691703	-0.375765
1	2.058889	-3.372077	0.219288
1	2.462545	-2.883728	-1.431856
1	3.733931	-2.901756	-0.180282
6	-2.878535	-0.818308	1.772777
1	-2.796088	0.216757	2.116388
1	-3.924933	-1.140221	1.836560
1	-2.269978	-1.441612	2.434438
6	-3.569427	-0.039707	-0.884098
1	-4.564713	-0.428382	-0.636927
1	-3.530515	1.024646	-0.633320
1	-3.409055	-0.141729	-1.962179
6	-2.671693	-2.695215	-0.373316
1	-2.458103	-2.888952	-1.428879
1	-2.055493	-3.374028	0.223499
1	-3.730553	-2.905763	-0.178368

Product Conctrans

ΔE_{gas} -3661.60293864
ΔE_{gas} (ZPE) -3661.335812
ΔG_{gas} -3661.386135

46	-0.000165	-0.475130	-0.000094
15	-2.347103	-0.405420	0.000002
15	2.347301	-0.381222	0.000028
6	0.069312	-2.549151	-0.000121
1	0.609191	-2.888058	-0.891402
1	0.607847	-2.888027	0.892000
1	-0.919311	-3.009837	-0.000878
35	-0.016168	2.123149	-0.000020
6	-3.044857	0.497542	-1.448467
1	-4.133036	0.592636	-1.364299
1	-2.585047	1.487362	-1.493873
1	-2.799805	-0.042036	-2.367788
6	-3.044510	0.497544	1.448642
1	-2.584896	1.487465	1.493777
1	-4.132745	0.592358	1.364894
1	-2.798954	-0.041878	2.367921
6	-3.338172	-1.966624	0.000156
1	-3.104112	-2.563580	0.886121
1	-4.408831	-1.735820	0.000558
1	-3.104762	-2.563397	-0.886107
6	3.040253	0.523544	-1.448908
1	2.576942	1.511818	-1.493641
1	4.128257	0.622014	-1.366787
1	2.795153	-0.016687	-2.367836
6	3.040073	0.523066	1.449347
1	4.128041	0.621911	1.367186
1	2.576490	1.511189	1.494583
1	2.795230	-0.017697	2.368032
6	3.332961	-1.944634	-0.000179
1	3.095039	-2.540788	-0.885236
1	4.404809	-1.719970	0.000126
1	3.094629	-2.541325	0.884405

Adduct S_N2cis

ΔE_{gas} -3661.55992608
ΔE_{gas}(ZPE) -3661.293506
ΔG_{gas} -3661.351182

6	1.570150	-2.329271	-0.023632
1	1.454420	-2.906772	-0.938662
1	1.443151	-2.953670	0.858552
1	0.900604	-1.464954	-0.005496
35	3.425256	-1.653778	0.005445
15	-2.803228	-0.858209	0.002461
46	-0.975593	0.547925	-0.002337
15	0.753986	2.091678	-0.000867
6	0.225822	3.870688	0.002927
1	-0.386549	4.071374	-0.880812
1	-0.385032	4.067769	0.888524
1	1.089903	4.546003	0.003584
6	1.930742	2.065738	1.432050
1	2.442789	1.099880	1.462537
1	2.677845	2.864705	1.352950
1	1.371955	2.187517	2.364434
6	1.930845	2.072233	-1.433880
1	2.678017	2.870719	-1.350891
1	2.442977	1.106579	-1.469101
1	1.372048	2.198642	-2.365649
6	-4.411191	-0.102696	-0.533296
1	-4.650116	0.742245	0.118690
1	-4.311994	0.277472	-1.553960
1	-5.231362	-0.829914	-0.497057
6	-3.295957	-1.612626	1.625272
1	-4.186790	-2.244318	1.524246
1	-2.470011	-2.215513	2.013603
1	-3.499010	-0.817186	2.347922
6	-2.754430	-2.366355	-1.080442

1	-1.921321	-3.007883	-0.778865
1	-3.687227	-2.939599	-1.017276
1	-2.588245	-2.063698	-2.118272

TS S_N2cis

ΔE_{gas} -3661.51498330
ΔE_{gas}(ZPE) -3661.250522
ΔG_{gas} -3661.303993

6	-1.248327	-1.403930	0.109249
1	-1.355137	-1.892373	1.081236
1	-1.338177	-2.124677	-0.706730
1	-1.989760	-0.567216	-0.012717
35	-4.163384	-0.084344	-0.026000
15	1.692132	-1.850790	-0.016439
46	0.296473	-0.066677	0.050664
15	1.230561	2.183306	-0.003491
6	2.775289	2.555591	-0.954737
1	3.619669	2.009284	-0.523991
1	2.652957	2.236503	-1.993823
1	3.001588	3.627452	-0.937141
6	0.022539	3.372721	-0.745394
1	-0.924635	3.322831	-0.200513
1	0.404485	4.399289	-0.714678
1	-0.177567	3.094376	-1.784000
6	1.588648	2.962299	1.636227
1	1.894384	4.007907	1.520851
1	0.692492	2.920551	2.261774
1	2.384580	2.411108	2.145246
6	3.475624	-1.404505	0.166377
1	3.763551	-0.707201	-0.624668
1	3.636159	-0.919519	1.133016
1	4.107663	-2.297904	0.104647
6	1.674440	-2.802403	-1.596139
1	2.419723	-3.605149	-1.572164
1	0.683341	-3.234398	-1.753789
1	1.892383	-2.132984	-2.432422
6	1.476961	-3.156905	1.266981
1	0.489341	-3.612612	1.165472
1	2.245504	-3.931084	1.165112
1	1.546696	-2.709915	2.262345

Product S_N2cis

ΔE_{gas} -3661.58886024
ΔE_{gas}(ZPE) -3661.321315
ΔG_{gas} -3661.371255

15	1.039846	1.677745	0.005832
46	-0.121720	-0.473611	0.020943
15	-2.348948	0.048568	-0.011003
35	2.212712	-1.471352	-0.025685
6	-3.299715	-0.496747	1.476980
1	-4.367236	-0.281243	1.357949
1	-3.162286	-1.567252	1.641238
1	-2.923109	0.033379	2.356466
6	-3.281167	-0.699504	-1.420191
1	-3.133300	-1.780695	-1.439447
1	-4.351238	-0.479502	-1.339532
1	-2.901003	-0.287146	-2.359244
6	-2.902301	1.809894	-0.141391
1	-3.996333	1.861026	-0.164794
1	-2.540833	2.385923	0.713509
1	-2.508844	2.261096	-1.055645
6	2.204288	1.845295	1.430239
1	2.847011	0.963094	1.458227
1	2.811918	2.752035	1.335148
1	1.634488	1.890360	2.363448
6	0.212846	3.342165	0.054896
1	-0.391585	3.441117	0.961022
1	0.965405	4.138496	0.052197
1	-0.438054	3.477068	-0.812894
6	2.135715	1.882968	-1.466889
1	2.750097	2.785766	-1.378087
1	2.774639	1.000855	-1.546461
1	1.523549	1.951927	-2.371357
6	-0.780493	-2.465269	0.069283
1	-0.238345	-2.923490	0.898892
1	-1.852592	-2.637843	0.197398
1	-0.446639	-2.909056	-0.872404

Adduct $S_N2trans$

ΔE_{gas} -3661.55994341
ΔE_{gas}(ZPE) -3661.293657
ΔG_{gas} -3661.351749

6	1.594654	-2.330224	-0.040916
1	1.490603	-2.901138	-0.961462
1	1.464284	-2.962534	0.835101
1	0.919372	-1.470539	-0.021484
35	3.444682	-1.642246	0.009619
15	-2.800539	-0.871562	0.003145
46	-0.972267	0.533532	-0.004382
15	0.736408	2.099621	-0.001416
6	1.902551	2.104438	1.440570
1	2.434677	1.149828	1.480182
1	2.633109	2.918670	1.362900
1	1.334300	2.219015	2.368117
6	1.925116	2.094405	-1.424978
1	2.655966	2.907612	-1.339954
1	2.455911	1.138624	-1.451263
1	1.371762	2.205476	-2.361945
6	0.175648	3.868620	-0.012771
1	-0.444725	4.060042	0.867439
1	1.026988	4.559950	-0.011010
1	-0.434589	4.051906	-0.901730
6	-4.448445	-0.040383	-0.192822
1	-4.469929	0.505401	-1.140308
1	-5.271230	-0.765396	-0.174968
1	-4.588486	0.682914	0.615448
6	-3.104600	-1.887343	1.527014
1	-3.199869	-1.224490	2.391754
1	-4.014488	-2.492568	1.434405
1	-2.250939	-2.548086	1.703512
6	-2.914041	-2.176819	-1.312648
1	-2.058115	-2.853265	-1.232830
1	-3.839719	-2.758332	-1.225391
1	-2.877808	-1.703985	-2.298222

TS $S_N2trans$

ΔE_{gas} -3661.53600970
ΔE_{gas}(ZPE) -3661.270623
ΔG_{gas} -3661.322900

6	1.197932	-0.337346	0.083251
1	1.323863	-0.214061	-0.982834
1	1.113092	-1.333384	0.486616
1	1.537048	0.439291	0.750855
35	3.720269	-0.927004	-0.011332
15	-1.731391	-1.979304	-0.006260
46	-0.997451	0.246398	0.013032
15	-0.486517	2.541351	-0.007378
6	0.858155	3.064904	-1.162171
1	1.044270	4.142046	-1.089632
1	1.781181	2.527422	-0.926838
1	0.574973	2.818398	-2.189425
6	0.079144	3.260775	1.600313
1	0.981169	2.742822	1.938601
1	0.300676	4.329162	1.500598
1	-0.696878	3.123024	2.358405
6	-1.873555	3.674267	-0.475364
1	-2.706759	3.544700	0.221215
1	-1.552338	4.721854	-0.458614
1	-2.226875	3.424935	-1.479891
6	-3.535891	-2.231652	-0.332747
1	-3.795698	-3.296342	-0.326161
1	-4.124295	-1.715250	0.430971
1	-3.794123	-1.807062	-1.307027
6	-0.946392	-3.080282	-1.267079
1	-1.326411	-4.104867	-1.188895
1	-1.155247	-2.695634	-2.269327
1	0.138396	-3.090322	-1.127966
6	-1.479887	-2.935442	1.557008
1	-1.836066	-3.966276	1.452974
1	-0.416757	-2.952340	1.813461
1	-2.018276	-2.449327	2.375362

Product $S_N2trans$

ΔE_{gas} -3661.53617792
ΔE_{gas}(ZPE) -3661.270187
ΔG_{gas} -3661.322472

35	-3.734131	-0.926512	-0.011400
15	0.478151	2.545744	-0.008821
46	1.036778	0.256083	0.014519
15	1.721486	-1.991341	-0.007305
6	0.903867	-3.048735	-1.281347
1	1.246179	-4.086829	-1.210672
1	-0.180881	-3.019794	-1.145754
1	1.131455	-2.662367	-2.278777
6	1.422280	-2.936740	1.551903
1	0.356850	-2.916335	1.797493
1	1.742893	-3.979072	1.448746
1	1.970427	-2.471078	2.375608
6	3.519777	-2.295091	-0.320798
1	4.118319	-1.799682	0.448982
1	3.746259	-3.367223	-0.314524
1	3.798906	-1.877729	-1.292451
6	1.834023	3.712789	-0.481253
1	1.483926	4.750966	-0.465967
1	2.671518	3.608714	0.214525
1	2.192112	3.472187	-1.486237
6	-0.884362	3.017421	-1.161852
1	-1.107763	4.087202	-1.088059
1	-0.592719	2.781596	-2.189188
1	-1.786762	2.446450	-0.925424
6	-0.102637	3.240231	1.602433
1	-0.360382	4.300492	1.504903
1	-0.985402	2.691535	1.942533
1	0.681078	3.127683	2.356741
6	-1.069606	-0.303617	0.091633
1	-1.497937	0.455279	0.733499
1	-1.286593	-0.226674	-0.967680
1	-1.073314	-1.300794	0.510397

2.1.1.4 PPh_3

$Pd(PPh_3)_2$

ΔE_{gas} -2200.57347484
ΔE_{gas}(ZPE) -2200.022779
ΔG_{gas} -2200.099436

46	-0.000257	0.003052	0.001513
15	-2.316837	0.000783	-0.000489
15	2.317466	0.000109	0.000016
6	-3.096161	-0.084725	1.675883
6	-2.459228	0.597664	2.726888
6	-4.275897	-0.794975	1.947032
6	-2.998701	0.584693	4.013848
1	-1.532383	1.131771	2.530849
6	-4.808410	-0.817921	3.239453
1	-4.779532	-1.336225	1.151729
6	-4.173994	-0.126451	4.273574
1	-2.495436	1.119374	4.814902
1	-5.720115	-1.376156	3.435102
1	-4.588977	-0.146241	5.277600
6	-3.097951	1.493883	-0.765798
6	-4.281212	2.079942	-0.289739
6	-2.459753	2.065239	-1.880557
6	-4.814427	3.210311	-0.916311
1	-4.786625	1.659486	0.574620
6	-2.999551	3.186286	-2.512409
1	-1.529852	1.632306	-2.242431
6	-4.177915	3.763112	-2.029580
1	-5.728357	3.656190	-0.532908
1	-2.494233	3.615522	-3.373360
1	-4.593399	4.642234	-2.514530
6	-3.093330	-1.410664	-0.910783
6	-2.454472	-2.660879	-0.841352
6	-4.272256	-1.294200	-1.663267
6	-2.990868	-3.771284	-1.494637
1	-1.527350	-2.754868	-0.280058
6	-4.802237	-2.404668	-2.327036
1	-4.777451	-0.335920	-1.737928
6	-4.165706	-3.644621	-2.241774
1	-2.485843	-4.731291	-1.429591
1	-5.713252	-2.297815	-2.909885
1	-4.578479	-4.506230	-2.759343
6	3.095568	1.629904	-0.404474
6	2.458654	2.791103	0.067494
6	4.272291	1.763034	-1.157885
6	2.994854	4.052910	-0.192455
1	1.533109	2.699739	0.631621
6	4.801851	3.028586	-1.427935
1	4.776577	0.880426	-1.539976
6	4.167716	4.174419	-0.943469
1	2.491269	4.940397	0.181264
1	5.711329	3.115855	-2.016403
1	4.580348	5.156959	-1.155597
6	3.097224	-0.463733	1.612889
6	2.461147	-1.451254	2.385273
6	4.276779	0.120066	2.099477
6	3.002151	-1.858233	3.605539
1	1.533196	-1.891734	2.027555
6	4.811531	-0.279992	3.327763
1	4.780540	0.889651	1.522525
6	4.178564	-1.270870	4.080914
1	2.499925	-2.624940	4.189339
1	5.724310	0.183413	3.692692
1	4.595269	-1.579917	5.035640
6	3.095003	-1.165601	-1.208531
6	4.284330	-1.866117	-0.953831
6	2.448687	-1.353795	-2.442645
6	4.816609	-2.731472	-1.914104
1	4.795237	-1.742436	-0.003662
6	2.986865	-2.209392	-3.404813
1	1.514659	-0.832494	-2.639233
6	4.172130	-2.902184	-3.141276
1	5.735768	-3.270693	-1.700953
1	2.475761	-2.342743	-4.354467
1	4.587073	-3.576127	-3.885821

Adduct Conccis

ΔE_{gas} -4811.90461933
ΔE_{gas}(ZPE) -4811.315775
ΔG_{gas} -4811.404538

6	-1.552445	3.606400	0.588164
1	-2.099299	3.700605	1.523630
1	-2.127341	3.064369	-0.157762
1	-0.573996	3.156733	0.740363
15	2.475558	-0.386783	-0.014460
46	0.189340	-0.752757	-0.056415
15	-2.100914	-1.053129	-0.032357
35	-1.261537	5.433189	-0.101922
6	3.418785	-1.463306	1.158334
6	2.761530	-1.891331	2.323991
6	4.743385	-1.872270	0.939516
6	3.419162	-2.693665	3.257216
1	1.725866	-1.601008	2.484804
6	5.396796	-2.684462	1.869647
1	5.264233	-1.564730	0.037580
6	4.738340	-3.093482	3.030927
1	2.897005	-3.015806	4.154373
1	6.421035	-2.997752	1.684210
1	5.248164	-3.726690	3.752320
6	3.361342	-0.626301	-1.621173
6	4.458510	0.150623	-2.023053
6	2.901279	-1.642819	-2.474935
6	5.085882	-0.089668	-3.248303
1	4.819220	0.950661	-1.383182
6	3.535687	-1.888586	-3.692891
1	2.034542	-2.230782	-2.181926
6	4.628906	-1.110886	-4.083107
1	5.931905	0.523204	-3.548692
1	3.168588	-2.679147	-4.342180
1	5.117013	-1.295180	-5.036532
6	2.955625	1.331377	0.479416
6	2.262990	2.397153	-0.123144
6	3.941049	1.621311	1.433485
6	2.558810	3.718874	0.209368
1	1.483461	2.183774	-0.850952
6	4.227742	2.946954	1.776180
1	4.483885	0.814334	1.915818
6	3.541167	3.996308	1.165573
1	2.011634	4.529080	-0.265093
1	4.990809	3.154743	2.522009
1	3.763895	5.025429	1.434352
6	-3.050407	0.264285	-0.924582
6	-2.491110	0.781486	-2.106342
6	-4.268625	0.790118	-0.468185
6	-3.140810	1.789490	-2.819783
1	-1.533572	0.399087	-2.452166
6	-4.913055	1.808489	-1.177339
1	-4.712192	0.415077	0.449162
6	-4.352903	2.309059	-2.354105
1	-2.694176	2.179762	-3.730359
1	-5.852716	2.210021	-0.806875
1	-4.852155	3.103672	-2.901800
6	-2.872293	-1.057983	1.650842
6	-3.985786	-1.839048	1.994568
6	-2.301707	-0.225461	2.629028
6	-4.521644	-1.780721	3.284238
1	-4.433852	-2.499379	1.257915
6	-2.845527	-0.158638	3.912263
1	-1.418370	0.357500	2.378278
6	-3.956899	-0.938446	4.243288
1	-5.381307	-2.396029	3.537149
1	-2.393983	0.492470	4.656326
1	-4.375127	-0.895025	5.245453
6	-2.720632	-2.620050	-0.795000
6	-3.899537	-2.701522	-1.551262
6	-1.955935	-3.783434	-0.603414
6	-4.307216	-3.921046	-2.098792
1	-4.497682	-1.811121	-1.720688
6	-2.371112	-5.002154	-1.139978
1	-1.027826	-3.722591	-0.039827
6	-3.547269	-5.073167	-1.891356
1	-5.219886	-3.967848	-2.687366
1	-1.770339	-5.893853	-0.981074
1	-3.865385	-6.020574	-2.318451

TS Conccis

ΔE_{gas} -4811.86266848
ΔE_{gas}(ZPE) -4811.275670
ΔG_{gas} -4811.358745

6	-0.444507	-2.515872	-1.978813
1	0.177069	-3.246654	-2.481216
1	-1.487472	-2.799594	-1.900162
1	-0.267746	-1.506475	-2.375477
15	2.116764	0.218967	-0.043189
46	-0.021887	-0.826055	-0.328568
15	-2.178451	0.117436	-0.044639
35	0.376062	-3.369476	0.039532
6	2.163118	2.056477	0.201891
6	1.229900	2.830390	-0.509200
6	3.057383	2.708275	1.065142
6	1.203772	4.219494	-0.376861
1	0.510872	2.337683	-1.158309
6	3.019852	4.097996	1.209634
1	3.781590	2.131707	1.631940
6	2.097651	4.857084	0.487088
1	0.474569	4.798536	-0.937279
1	3.715061	4.585730	1.888330
1	2.070672	5.937570	0.601554
6	3.114067	-0.428182	1.373297
6	4.517591	-0.475884	1.371975
6	2.422239	-0.902348	2.499807
6	5.211520	-0.975837	2.475968
1	5.070593	-0.129883	0.503271
6	3.117575	-1.395094	3.605745
1	0.474569	4.798536	-0.937279
1	3.715061	4.585730	1.888330
1	2.070672	5.937570	0.601554
6	3.114067	-0.428182	1.373297
6	4.517591	-0.475884	1.371975
6	2.422239	-0.902348	2.499807
6	5.211520	-0.975837	2.475968
1	5.070593	-0.129883	0.503271
6	3.117575	-1.395094	3.605745
1	1.335479	-0.902358	2.498181
6	4.513363	-1.433153	3.595873
1	6.297939	-1.009325	2.458949
1	2.566820	-1.761823	4.467940
1	5.054735	-1.825508	4.452764
6	3.250351	-0.036661	-1.487682
6	3.463799	-1.360270	-1.916551
6	3.853300	1.008311	-2.202104
6	4.271622	-1.627975	-3.020784
1	2.993066	-2.180873	-1.380196
6	4.651131	0.737344	-3.318873
1	3.700832	2.037230	-1.891794
6	4.864995	-0.578253	-3.729468
1	4.433404	-2.656912	-3.331914
1	5.108986	1.559982	-3.862458
1	5.488094	-0.786799	-4.595134
6	-3.626993	-0.994028	-0.376427
6	-3.523899	-2.334452	0.039331
6	-4.791778	-0.585605	-1.044569
6	-4.566493	-3.233792	-0.189383
1	-2.619218	-2.675704	0.537114
6	-5.828420	-1.491814	-1.285752
1	-4.893251	0.441900	-1.379489
6	-5.721067	-2.815423	-0.856464
1	-4.470299	-4.263565	0.144688
1	-6.721692	-1.158458	-1.807946
1	-6.528759	-3.517965	-1.044006
6	-2.601611	1.630264	-1.030684
6	-3.382466	2.684332	-0.531483
6	-2.104483	1.724787	-2.341137
6	-3.658766	3.801830	-1.323691
1	-3.770123	2.637220	0.481764
6	-2.389601	2.835406	-3.136868
1	-1.479435	0.926173	-2.733507

6	-3.165987	3.879527	-2.627739
1	-4.261286	4.611291	-0.919441
1	-1.997880	2.889120	-4.149411
1	-3.381754	4.749504	-3.242345
6	-2.469185	0.674227	1.698014
6	-3.581145	0.285476	2.459444
6	-1.501370	1.504874	2.291873
6	-3.721097	0.714550	3.783021
1	-4.338869	-0.358271	2.024509
6	-1.651838	1.944800	3.606437
1	-0.627204	1.806691	1.721314
6	-2.760655	1.546284	4.358871
1	-4.586707	0.398846	4.359840
1	-0.897145	2.592067	4.045626
1	-2.872234	1.880583	5.386945

Product Conccis

ΔE_{gas} -4811.91869522
ΔE_{gas}(ZPE) -4811.328237
ΔG_{gas} -4811.404587

6	-1.353945	-2.572475	-1.686055
1	-0.882138	-2.769144	-2.651676
1	-1.357841	-3.486339	-1.090016
1	-2.376125	-2.216847	-1.828665
15	1.777850	0.219887	0.096781
46	-0.042063	-1.226085	-0.749285
15	-1.968193	-0.056304	-0.161978
35	1.659093	-3.066673	-1.084525
6	1.667965	2.045804	-0.201604
6	0.979438	2.471805	-1.347696
6	2.351326	3.001219	0.566879
6	0.962391	3.820447	-1.712196
1	0.451305	1.743364	-1.957801
6	2.320485	4.350886	0.212823
1	2.912503	2.694245	1.444037
6	1.626667	4.764569	-0.927359
1	0.427077	4.130259	-2.605939
1	2.849046	5.078565	0.823222
1	1.611821	5.814917	-1.205918
6	1.962910	-0.033995	1.910703
6	2.542987	-1.240355	2.347178
6	1.416088	0.839221	2.863411
6	2.608011	-1.540558	3.707404
1	2.928256	-1.948623	1.619226
6	1.483051	0.531370	4.225144
1	0.926475	1.755654	2.551635
6	2.084201	-0.653034	4.651586
1	3.065735	-2.472645	4.027789
1	1.058701	1.221699	4.949339
1	2.138304	-0.888108	5.711332
6	3.475832	-0.052616	-0.588606
6	3.605675	-0.352888	-1.952564
6	4.633219	0.139298	0.179028
6	4.868377	-0.453433	-2.536850
1	2.719972	-0.535730	-2.552073
6	5.896640	0.026202	-0.405581
1	4.555779	0.367106	1.237744
6	6.016927	-0.267355	-1.764642
1	4.952785	-0.696203	-3.592610
1	6.785050	0.168217	0.204384
1	7.000302	-0.356871	-2.218634
6	-3.244133	-1.230200	0.490833
6	-2.801586	-2.307548	1.276699
6	-4.618495	-1.076462	0.264144
6	-3.717021	-3.197355	1.840330
1	-1.736366	-2.461953	1.428686
6	-5.531994	-1.976958	0.818329
1	-4.984695	-0.265039	-0.355588
6	-5.085292	-3.034559	1.611343
1	-3.357398	-4.025466	2.444934
1	-6.593773	-1.850530	0.624078
1	-5.797607	-3.734090	2.040268
6	-2.766799	0.839912	-1.565722
6	-3.788889	1.786819	-1.376851
6	-2.333517	0.565627	-2.872721
6	-4.370695	2.429947	-2.470323
1	-4.121868	2.036501	-0.373898
6	-2.917961	1.209674	-3.965567
1	-1.534834	-0.153428	-3.029009
6	-3.938617	2.140580	-3.767010
1	-5.159039	3.160036	-2.307445
1	-2.572064	0.982781	-4.970316
1	-4.392213	2.643126	-4.617034
6	-1.934068	1.222173	1.185716
6	-2.217250	0.871655	2.516135
6	-1.591268	2.555511	0.903929
6	-2.167648	1.828392	3.532028
1	-2.488918	-0.147968	2.765936
6	-1.539453	3.509772	1.921279
1	-1.366183	2.859145	-0.111295
6	-1.829039	3.150252	3.239556
1	-2.399449	1.535473	4.552465
1	-1.272862	4.534421	1.677408
1	-1.795054	3.895123	4.030140

Adduct Conctrans

ΔE_{gas} -4811.90554018
ΔE_{gas}(ZPE) -4811.316556
ΔG_{gas} -4811.404217

6	0.781266	-3.213212	-1.279644
1	1.850563	-3.212538	-1.474877
1	0.213387	-3.535690	-2.149423
1	0.441381	-2.241780	-0.918644
15	2.241974	0.655400	0.008313
46	-0.062807	0.479597	-0.050454
15	-2.381326	0.441413	-0.007179
35	0.448734	-4.529365	0.156671
6	3.145639	-0.289327	-1.304757
6	2.634339	-0.231705	-2.613486
6	4.272094	-1.086295	-1.055170
6	3.245129	-0.939486	-3.648516
1	1.743985	0.360355	-2.812205
6	4.875298	-1.807496	-2.090958
1	4.676634	-1.153598	-0.050104
6	4.366787	-1.734062	-3.388478
1	2.839198	-0.881125	-4.655101
1	5.743928	-2.425701	-1.879528
1	4.836698	-2.294714	-4.192121
6	3.019480	0.064170	1.579577
6	4.171824	0.636950	2.138958
6	2.412037	-1.018982	2.237415
6	4.707924	0.132377	3.326568
1	4.648672	1.482779	1.652593
6	2.956308	-1.529571	3.416471
1	1.504342	-1.453524	1.825782
6	4.104824	-0.953119	3.964752
1	5.597639	0.589874	3.751721
1	2.476145	-2.370288	3.909923
1	4.523930	-1.343981	4.888243
6	2.899719	2.373477	-0.188722
6	2.133029	3.431015	0.328525
6	4.116555	2.666988	-0.823619
6	2.581413	4.748442	0.228966
1	1.175693	3.212731	0.795940
6	4.558671	3.988006	-0.932328
1	4.717410	1.864758	-1.242114
6	3.794809	5.030079	-0.403681
1	1.977159	5.555479	0.635011
6	5.500942	4.200515	-1.430909
1	4.139589	6.057133	-0.490340
6	-3.161359	1.966029	-0.710561
6	-2.470471	2.643078	-1.729316
6	-4.394282	2.475790	-0.275244
6	-3.008462	3.791681	-2.311954
1	-1.499975	2.269729	-2.048188
6	-4.926231	3.631717	-0.851327
1	-4.936881	1.976592	0.521908
6	-4.237260	4.289369	-1.872570
1	-2.461595	4.303574	-3.099489
1	-5.879507	4.018175	-0.499871
1	-4.652534	5.189454	-2.318341
6	-3.122302	0.315451	1.683298
6	-4.354836	-0.304065	1.942616
6	-2.408419	0.879171	2.753500
6	-4.865335	-0.349012	3.242185
1	-4.912847	-0.762324	1.131218
6	-2.924211	0.841685	4.049517
1	-1.438629	1.332703	2.561966
6	-4.153819	0.226592	4.296641
1	-5.818969	-0.836111	3.429004
1	-2.359901	1.282274	4.867292
1	-4.551566	0.188487	5.307377
6	-3.206377	-0.937616	-0.925824
6	-2.811543	-2.252936	-0.621959
6	-4.162573	-0.735934	-1.931265
6	-3.371087	-3.337641	-1.296086
1	-2.058101	-2.430705	0.141411
6	-4.713242	-1.824700	-2.615459
1	-4.479313	0.270561	-2.185848
6	-4.322776	-3.125663	-2.298895
1	-3.055066	-4.345936	-1.042028
1	-5.450974	-1.650157	-3.394569
1	-4.753127	-3.970341	-2.830328

TS Conctrans

ΔE_{gas} -4811.86177829
ΔE_{gas}(ZPE) -4811.274594
ΔG_{gas} -4811.356929

6	-0.061073	-2.190844	-2.075527
1	0.806213	-2.742604	-2.416210
1	-1.014192	-2.642249	-2.322440
1	-0.010469	-1.123158	-2.336147
15	2.218534	0.219743	-0.039993
46	-0.000581	-0.640984	-0.269600
15	-2.225189	0.200435	-0.033729
35	0.048686	-3.239945	0.017682
6	3.483142	-0.652802	-1.077425
6	3.326248	-0.619879	-2.475514
6	4.534460	-1.409771	-0.540768
6	4.204316	-1.308825	-3.311092
1	2.511880	-0.046510	-2.913322
6	5.407741	-2.110245	-1.379179
1	4.673805	-1.458433	0.534397
6	5.248636	-2.060768	-2.763831
1	4.070952	-1.262503	-4.388974
1	6.215449	-2.692876	-0.943673
1	5.929581	-2.604209	-3.413307
6	2.882888	0.047525	1.682044
6	3.762220	0.972668	2.265994
6	2.467292	-1.061270	2.439647
6	4.217150	0.791454	3.574352
1	4.090159	1.840632	1.702733
6	2.933258	-1.246490	3.742493
1	1.774771	-1.777160	2.005179
6	3.806793	-0.318785	4.314675
1	4.893488	1.520566	4.013330
1	2.604700	-2.112119	4.311936
1	4.161985	-0.457894	5.332439
6	2.546824	2.000821	-0.434795
6	1.516500	2.923134	-0.193503
6	3.767119	2.471285	-0.947467
6	1.704171	4.283738	-0.442543
1	0.559290	2.565691	0.175917
6	3.950454	3.831506	-1.207008
1	4.574690	1.774386	-1.151271
6	2.921373	4.740807	-0.952181
1	0.892430	4.980878	-0.252760
1	4.899488	4.179549	-1.607059
1	3.065916	5.798653	-1.156031
6	-2.521492	1.981132	-0.461533
6	-1.864976	2.498842	-1.591188
6	-3.344567	2.837377	0.285997
6	-2.042527	3.827997	-1.976468
1	-1.199346	1.856212	-2.162450
6	-3.507655	4.173911	-0.089045

1	-3.857699	2.464212	1.166704
6	-2.862797	4.671506	-1.222580
1	-1.528328	4.207430	-2.855608
1	-4.143543	4.824302	0.506238
1	-2.993462	5.710380	-1.513954
6	-2.881248	0.060668	1.691244
6	-4.243052	-0.120240	1.982470
6	-1.967397	0.140558	2.754631
6	-4.679543	-0.211301	3.305966
1	-4.963867	-0.198932	1.173787
6	-2.406172	0.058213	4.077287
1	-0.907698	0.252134	2.539344
6	-3.763001	-0.119039	4.355720
1	-5.736423	-0.355506	3.515312
1	-1.685530	0.121531	4.888434
1	-4.104104	-0.191906	5.385099
6	-3.526030	-0.671835	-1.028564
6	-3.584755	-2.075227	-0.932939
6	-4.407862	-0.020719	-1.903853
6	-4.511050	-2.801349	-1.681605
1	-2.898319	-2.600725	-0.273574
6	-5.326813	-0.752758	-2.662982
1	-4.381389	1.060265	-1.996930
6	-5.383656	-2.142040	-2.552900
1	-4.545699	-3.883768	-1.588448
1	-6.001452	-0.230637	-3.336818
1	-6.100266	-2.708707	-3.141486

Product Conctrans

ΔE_{gas} -4811.93067621
ΔE_{gas}(ZPE) -4811.340718
ΔG_{gas} -4811.419727

6	0.012366	2.125042	0.467610
1	-0.481072	2.647065	-0.357723
1	-0.563884	2.288675	1.382887
1	1.008743	2.549263	0.601515
46	0.014850	0.084347	0.024629
15	2.382896	0.200376	0.037041
15	-2.373291	0.104987	0.032632
35	-0.038478	-2.440856	-0.476852
6	3.372736	-1.193806	-0.653480
6	3.351058	-2.428958	0.016859
6	4.119362	-1.073267	-1.834171
6	4.077131	-3.511309	-0.476543
1	2.758745	-2.548027	0.917464
6	4.838179	-2.164472	-2.330351
1	4.148873	-0.130256	-2.369620
6	4.820899	-3.383092	-1.652537
1	4.049864	-4.459779	0.052629
1	5.413863	-2.054877	-3.245627
1	5.381020	-4.230621	-2.038614
6	2.993923	1.668797	-0.904441
6	4.039562	2.493056	-0.467060
6	2.361109	1.964520	-2.123760
6	4.449531	3.584558	-1.237803
1	4.531329	2.294860	0.479628
6	2.779776	3.046944	-2.897635
1	1.528217	1.350738	-2.457618
6	3.825498	3.861141	-2.454710
1	5.256754	4.219184	-0.881781
1	2.281682	3.260347	-3.839591
1	4.145990	4.710586	-3.051830
6	3.066392	0.369496	1.743652
6	4.430097	0.162790	2.016439
6	2.205475	0.693315	2.803247
6	4.920769	0.297538	3.315709
1	5.107158	-0.118868	1.215233
6	2.698660	0.824834	4.103378
1	1.146750	0.829112	2.607006
6	4.056252	0.631124	4.361446
1	5.977152	0.133833	3.511442
1	2.018110	1.072511	4.913557
1	4.438986	0.730069	5.373733
6	-3.114447	-0.744659	-1.427500
6	-2.387440	-0.776358	-2.626863
6	-4.390793	-1.323589	-1.387428
6	-2.935925	-1.358567	-3.770448
1	-1.379960	-0.372654	-2.654174
6	-4.932617	-1.915591	-2.529794
1	-4.959497	-1.328197	-0.463073
6	-4.209006	-1.929966	-3.723737
1	-2.358401	-1.383618	-4.690516
1	-5.918784	-2.369922	-2.483053
1	-4.630897	-2.394608	-4.610978
6	-3.125554	-0.692192	1.519910
6	-4.422362	-0.373178	1.960457
6	-2.388720	-1.659619	2.221885
6	-4.967847	-1.007944	3.077412
1	-5.005252	0.380202	1.439769
6	-2.939782	-2.292397	3.338225
1	-1.397363	-1.933382	1.875497
6	-4.226918	-1.968371	3.769629
1	-5.971270	-0.749513	3.405597
1	-2.358129	-3.042533	3.867217
1	-4.652114	-2.461207	4.640046
6	-3.181382	1.769486	-0.008359
6	-3.641774	2.321567	-1.213866
6	-3.255086	2.550336	1.158658
6	-4.171319	3.613746	-1.249336
1	-3.597026	1.740304	-2.129182
6	-3.789047	3.838798	1.122103
1	-2.905362	2.147468	2.104694
6	-4.248454	4.375473	-0.082929
1	-4.528500	4.020017	-2.191919
1	-3.844184	4.422838	2.036919
1	-4.663784	5.379205	-0.110938

Adduct S_N2trans

ΔE_{gas} -4811.90462205
ΔE_{gas}(ZPE) -4811.315639
ΔG_{gas} -4811.403922

6	0.837944	3.415253	-0.917630
1	1.901636	3.520593	-0.718807
1	0.469507	2.443292	-0.588769
1	0.602826	3.598707	-1.963936
35	-0.092579	4.800684	0.137664
15	-2.327446	-0.546779	-0.012000
46	-0.007939	-0.461653	-0.043093
15	2.300288	-0.577177	0.001531
6	3.154580	0.910734	0.698013
6	4.337561	1.449829	0.170654
6	2.551763	1.547421	1.796964
6	4.905686	2.598073	0.731291
1	4.814245	0.980426	-0.684454
6	3.126187	2.685510	2.363392
1	1.617110	1.156659	2.192554
6	4.304233	3.216209	1.828851
1	5.819068	3.007458	0.307336
1	2.644265	3.168247	3.209119
1	4.744632	4.110558	2.261306
6	3.114816	-0.812827	-1.643562
6	4.302663	-1.537973	-1.823436
6	2.500779	-0.231020	-2.765650
6	4.868247	-1.668198	-3.094590
1	4.784285	-2.010137	-0.972066
6	3.072954	-0.351865	-4.032697
1	1.561441	0.302450	-2.639013
6	4.258215	-1.072300	-4.199920
1	5.785914	-2.237407	-3.218895
1	2.586641	0.106055	-4.890135
1	4.699267	-1.175545	-5.187836
6	2.973798	-1.970889	1.015114
6	4.119564	-1.863766	1.817773
6	2.286225	-3.196022	0.975400
6	4.570275	-2.959821	2.558960
1	4.657960	-0.922324	1.873496
6	2.745093	-4.292175	1.705586
1	1.380738	-3.278281	0.378872
6	3.887806	-4.175783	2.501594
1	5.456327	-2.860031	3.180704
1	2.203169	-5.233332	1.662579
1	4.239455	-5.026457	3.079420
6	-3.006747	-2.161192	-0.613279
6	-2.295175	-2.837739	-1.618322
6	-4.185192	-2.737057	-0.114869
6	-2.760530	-4.051972	-2.125065
1	-1.366804	-2.409906	-1.989485
6	-4.643267	-3.958741	-0.614357
1	-4.743058	-2.236860	0.671010
6	-3.934962	-4.616574	-1.621826
1	-2.199364	-4.561599	-2.904023
1	-5.554728	-4.395456	-0.214194
1	-4.292712	-5.567423	-2.008123
6	-3.091187	-0.357845	1.662195
6	-4.347301	0.229804	1.876961
6	-2.369984	-0.840712	2.766775
6	-4.872497	0.325869	3.168100
1	-4.913021	0.621407	1.036616
6	-2.901126	-0.754330	4.054038
1	-1.384609	-1.272914	2.608026
6	-4.153174	-0.168844	4.257577
1	-5.844375	0.788264	3.320420
1	-2.332269	-1.134083	4.898782
1	-4.562848	-0.092010	5.261329
6	-3.228265	0.708425	-1.031078
6	-4.184377	0.375221	-2.001202
6	-2.897852	2.062688	-0.844622
6	-4.797270	1.373653	-2.765345
1	-4.451855	-0.663623	-2.166605
6	-3.518526	3.057474	-1.598979
1	-2.149565	2.343194	-0.107816
6	-4.469290	2.714456	-2.565330
1	-5.533897	1.097596	-3.515641
1	-3.249256	4.097496	-1.435745
1	-4.947294	3.488572	-3.159829

TS S_N2trans

ΔE_{gas} -4811.88030854
ΔE_{gas}(ZPE) -4811.292294
ΔG_{gas} -4811.376161

6	0.106815	2.069418	0.059169
1	-0.923560	2.389608	0.040215
1	0.663723	2.128080	-0.865458
1	0.639268	2.111763	0.998446
35	0.645288	4.641935	0.057871
15	2.291124	-0.539188	-0.001767
46	-0.054447	-0.165529	0.017423
15	-2.399163	-0.293206	0.003064
6	-3.318467	1.092122	-0.789529
6	-4.519780	1.603007	-0.275549
6	-2.773948	1.667051	-1.950343
6	-5.164522	2.664764	-0.914726
1	-4.948690	1.180622	0.627925
6	-3.422697	2.723488	-2.589106
1	-1.829852	1.297485	-2.342516
6	-4.618810	3.225414	-2.070445
1	-6.090083	3.057107	-0.502235
1	-2.982157	3.167543	-3.476985
1	-5.115639	4.059144	-2.558580
6	-3.135121	-0.434606	1.688318
6	-4.219559	-1.276074	1.979668
6	-2.579106	0.343592	2.718205
6	-4.738810	-1.334450	3.275446
1	-4.656727	-1.890015	1.197898
6	-3.107388	0.291414	4.008164
1	-1.728786	0.987285	2.508925
6	-4.186554	-0.550157	4.289751
1	-5.576557	-1.992906	3.489327
1	-2.670697	0.902609	4.793143
1	-4.592451	-0.596878	5.296637
6	-2.988185	-1.802134	-0.882218
6	-4.103826	-1.800347	-1.732637
6	-2.272392	-2.998475	-0.702199
6	-4.495932	-2.971894	-2.386034
1	-4.663632	-0.883991	-1.891588

6	-2.671793	-4.168334	-1.347685
1	-1.395330	-3.010452	-0.059217
6	-3.783972	-4.156629	-2.193826
1	-5.359894	-2.955044	-3.045065
1	-2.108724	-5.085571	-1.197792
1	-4.090177	-5.065771	-2.704147
6	2.615824	-2.320360	0.364073
6	1.840723	-2.944183	1.357639
6	3.583571	-3.075713	-0.314508
6	2.040622	-4.288391	1.674856
1	1.078704	-2.371589	1.882026
6	3.772439	-4.424684	-0.004378
1	4.186959	-2.613877	-1.089543
6	3.005029	-5.032707	0.990722
1	1.438728	-4.754447	2.450474
1	4.522531	-4.998900	-0.541664
1	3.155140	-6.081902	1.230373
6	3.088561	-0.246105	-1.636398
6	4.440960	0.104101	-1.773592
6	2.303078	-0.397611	-2.790995
6	4.994935	0.292874	-3.041408
1	5.058795	0.241730	-0.891395
6	2.861194	-0.215662	-4.056732
1	1.250043	-0.650788	-2.690673
6	4.207926	0.131550	-4.183645
1	6.041379	0.570462	-3.134570
1	2.241700	-0.334033	-4.941606
1	4.640640	0.284273	-5.168596
6	3.345269	0.384222	1.197604
6	4.019878	-0.254826	2.249527
6	3.418901	1.785746	1.091847
6	4.752894	0.492184	3.175551
1	3.974355	-1.334255	2.351386
6	4.153036	2.525607	2.018636
1	2.905275	2.317803	0.296378
6	4.820886	1.881392	3.063144
1	5.271478	-0.017458	3.983455
1	4.185987	3.606945	1.923567
1	5.388244	2.460302	3.786838

Product $S_N2$trans

ΔE_{gas} -4811.88039193

ΔE_{gas}(ZPE) -4811.291787

ΔG_{gas} -4811.376310

6	-0.092605	-1.966501	0.040701
1	0.914169	-2.359259	-0.011676
1	-0.686352	-2.100578	-0.855859
1	-0.601271	-2.083711	0.989778
35	-0.731357	-4.654844	0.051159
15	-2.289038	0.554020	-0.000171
46	0.065601	0.195617	0.005540
15	2.413760	0.276865	0.000813
6	3.297809	-1.045871	-0.922637
6	4.534008	-1.562128	-0.505105
6	2.698387	-1.561619	-2.083787
6	5.159952	-2.570583	-1.240908
1	5.003111	-1.186924	0.399191
6	3.328160	-2.566324	-2.818341
1	1.727018	-1.189766	-2.399318
6	4.559448	-3.073182	-2.396511
1	6.113005	-2.968806	-0.903651
1	2.845715	-2.967564	-3.704774
1	5.041858	-3.867300	-2.959424
6	3.159034	0.248643	1.686302
6	4.245119	1.058234	2.052382
6	2.613023	-0.633073	2.635045
6	4.776851	0.983044	3.342164
1	4.674131	1.750889	1.334539
6	3.153722	-0.712752	3.918351
1	1.763382	-1.256219	2.369821
6	4.235036	0.097059	4.275004
1	5.616352	1.617082	3.614759
1	2.725248	-1.403215	4.639396
1	4.651034	0.039614	5.277162
6	3.007453	1.855988	-0.745279
6	4.053745	1.912799	-1.677669
6	2.356641	3.047628	-0.379421
6	4.441930	3.136957	-2.229439
1	4.563657	1.002855	-1.977848

6	2.752918	4.268427	-0.924036
1	1.534631	3.018780	0.332300
6	3.795579	4.315089	-1.853632
1	5.252300	3.165848	-2.952889
1	2.241670	5.181023	-0.629928
1	4.098932	5.265098	-2.284979
6	-2.586764	2.337422	0.372866
6	-1.838313	2.931421	1.405084
6	-3.501894	3.125100	-0.340857
6	-2.013308	4.278298	1.724488
1	-1.118722	2.333514	1.960471
6	-3.665333	4.476852	-0.027540
1	-4.085001	2.685900	-1.144024
6	-2.925146	5.055158	1.004999
1	-1.433943	4.720988	2.530346
1	-4.375022	5.076224	-0.591477
1	-3.055883	6.106333	1.247155
6	-3.091638	0.272200	-1.632243
6	-4.445049	-0.076898	-1.760656
6	-2.314028	0.429643	-2.791248
6	-5.008253	-0.258375	-3.025361
1	-5.055632	-0.219422	-0.874249
6	-2.881533	0.254795	-4.053680
1	-1.260045	0.681538	-2.698225
6	-4.229386	-0.091100	-4.172298
1	-6.055240	-0.535643	-3.112401
1	-2.268560	0.377137	-4.942499
1	-4.669235	-0.238619	-5.154843
6	-3.337878	-0.367122	1.202944
6	-4.052049	0.281055	2.223047
6	-3.380307	-1.771823	1.124222
6	-4.793549	-0.461074	3.145947
1	-4.030832	1.363059	2.302930
6	-4.122996	-2.506046	2.048819
1	-2.836125	-2.314070	0.356365
6	-4.830213	-1.853590	3.061676
1	-5.342819	0.054677	3.929314
1	-4.129877	-3.589517	1.975707
1	-5.404064	-2.428558	3.783436

2.1.2 Species Optimized in THF

ΔE_{THF} -2611.32866184
ΔE_{THF}(ZPE) -2611.291474
ΔG_{THF} -2611.315369

6	0.000000	0.000000	-1.550099
35	0.000000	0.000000	0.426228
1	0.000000	1.038299	-1.872463
1	0.899193	-0.519149	-1.872463
1	-0.899193	-0.519149	-1.872463

2.1.2.1 PF_3

$Pd(PF_3)_2$

ΔE_{THF} -1409.96501923
ΔE_{THF}(ZPE) -1409.946595
ΔG_{THF} -1409.988847

46	0.000046	-0.710899	-0.000021
15	-2.061995	0.151144	-0.000017
15	2.061913	0.151181	-0.000007
9	3.101571	-0.095309	-1.206139
9	3.101258	-0.094872	1.206482
9	2.174132	1.754952	-0.000291
9	-2.173960	1.754889	-0.000413
9	-3.101305	-0.094728	1.206557
9	-3.101797	-0.095324	-1.206048

Adduct Conccis

ΔE_{THF} -4021.30515249
ΔE_{THF}(ZPE) -4021.248883
ΔG_{THF} -4021.303457

15	2.227276	-0.664348	-0.012566
46	0.099065	0.023256	0.025611
15	-0.533023	2.163742	-0.006767
35	-1.699625	-1.978194	0.003537
6	-3.534969	-1.221691	-0.047179
1	-4.212919	-2.071707	-0.058459
1	-3.650390	-0.621413	0.851024
1	-3.608093	-0.628543	-0.954192
9	2.891749	-1.348517	1.288909
9	2.781922	-1.726001	-1.095052
9	3.395335	0.421688	-0.244406
9	0.523628	3.266940	-0.523579
9	-0.901758	2.908901	1.375469
9	-1.780065	2.735646	-0.864363

TS Conccis

ΔE_{THF} -4021.25841831
ΔE_{THF}(ZPE) -4021.203608
ΔG_{THF} -4021.253427

15	-1.409418	1.673634	0.024530
46	0.021743	-0.165554	0.152402
15	2.250814	0.280105	-0.104119
35	-1.306676	-2.238437	-0.414291
6	0.103675	-2.042595	1.588101
1	-0.737713	-2.523623	2.065655
1	0.893420	-2.706605	1.259944
1	0.430266	-1.146756	2.128074
9	-2.927942	1.568987	-0.494290
9	-1.722240	2.455437	1.394235
9	-1.005285	2.960060	-0.850312
9	2.872130	1.685889	0.370921
9	2.788667	0.336489	-1.615966
9	3.428504	-0.641615	0.495551

Product Conccis

ΔE_{THF} -4021.30360467
ΔE_{THF}(ZPE) -4021.246442
ΔG_{THF} -4021.293984

15	-0.904280	1.683983	-0.000149
46	0.098768	-0.480672	-0.000459
15	2.268586	-0.021013	0.000138
35	-2.264834	-1.343786	0.000374
6	0.714794	-2.489840	-0.000585
1	0.255369	-2.894400	-0.902217
1	1.790722	-2.664185	-0.003641
1	0.260591	-2.893086	0.904308
9	-1.868825	2.049605	-1.207728
9	-1.866591	2.050099	1.209080
9	-0.022858	3.013489	-0.001235
9	3.156548	-0.547468	-1.203641
9	3.156148	-0.550040	1.203071
9	2.741784	1.494269	0.001923

Adduct Conctrans

ΔE_{THF} -4021.30511535
ΔE_{THF}(ZPE) -4021.248691
ΔG_{THF} -4021.301711

15	-0.513117	2.133127	-0.005468
46	0.104730	-0.010403	0.016606
15	2.239696	-0.678859	-0.008641
35	-1.751389	-1.947046	0.009660
6	-3.546511	-1.098392	-0.054461
9	2.776034	-2.205323	-0.050236
9	3.191419	-0.205993	1.202827
9	3.177403	-0.147753	-1.206540
9	-1.754310	2.708463	-0.868079
9	-0.895684	2.862368	1.381799
9	0.543840	3.244660	-0.500802
1	-4.262616	-1.911104	-0.149896
1	-3.670011	-0.552087	0.876683
1	-3.554273	-0.443106	-0.921063

TS Conctrans

ΔE_{THF} -4021.25835279
ΔE_{THF}(ZPE) -4021.203691
ΔG_{THF} -4021.253677

15	2.060350	-1.004639	-0.055732
46	0.001475	0.045902	-0.023604
15	-2.060644	-1.008456	-0.057949
35	-0.010719	2.542094	-0.348869
6	0.015177	1.442492	1.876261
1	0.939768	1.960791	2.091523
1	-0.891410	1.983967	2.109770
1	0.003184	0.394862	2.192803
9	-3.305100	-0.394978	-0.872222
9	-2.822295	-1.219197	1.342284
9	-2.225427	-2.514691	-0.598256
9	3.193214	-0.527008	-1.092019
9	2.968435	-0.972999	1.271184
9	2.209961	-2.580343	-0.345441

Product Conctrans

ΔE_{THF} -4021.30235854
ΔE_{THF}(ZPE) -4021.245161
ΔG_{THF} -4021.293331

46	0.002805	-0.430880	-0.079012
15	-2.277060	-0.416533	0.043199
15	2.286377	-0.382653	0.044048
6	0.067454	-2.521551	-0.170114
1	0.653896	-2.776097	-1.055873
1	0.554875	-2.885121	0.736811
1	-0.934154	-2.938770	-0.251614
35	-0.032350	2.143700	-0.039941
9	-3.120713	-1.762448	0.023989
9	-3.075889	0.379033	-1.067425
9	-2.905029	0.240001	1.339051
9	3.076772	0.410897	-1.074028
9	2.909530	0.290479	1.333527
9	3.135785	-1.723731	0.035458

Adduct $S_N2$trans

ΔE_{THF} -4021.29392083
ΔE_{THF}(ZPE) -4021.237421
ΔE_{THF} -4021.286633

6	-2.700988	-1.358620	0.079916
1	-2.172931	-0.950539	0.939366
1	-2.904691	-2.419249	0.204197
1	-2.170404	-1.160975	-0.848770
35	-4.441856	-0.432484	-0.030013
15	2.151979	-1.698617	-0.019955
46	0.682763	-0.009961	0.068003
15	0.887503	2.212892	-0.006461
9	2.385835	2.791545	-0.059651
9	0.371038	3.177833	1.174894
9	0.319100	3.081647	-1.236843
9	3.084247	-1.953655	1.264444
9	3.337819	-1.562179	-1.095572
9	1.826358	-3.250360	-0.320129

TS $S_N2$trans

ΔE_{THF} -4021.25298218
ΔE_{THF}(ZPE) -4021.197777
ΔG_{THF} -4021.247672

6	-1.161215	-0.164506	-0.071146
1	-1.274591	-0.080945	1.002429
1	-1.209633	-1.141439	-0.527935
1	-1.413277	0.678737	-0.697781
35	-3.810068	-0.455378	0.008696
15	1.415909	-2.162363	0.002841
46	1.111132	0.131497	0.000301
15	0.805002	2.435422	-0.002244
9	0.340738	3.128597	1.360234
9	-0.285198	3.075646	-0.979456
9	2.034691	3.380849	-0.353791
9	1.359521	-2.945199	1.391490
9	2.786930	-2.746959	-0.555634
9	0.406811	-3.079135	-0.826949

2.1.2.2 PH_3

$Pd(PH_3)_2$

ΔE_{THF} -814.281202339
ΔE_{THF}(ZPE) -814.227508
ΔG_{THF} -814.259215

46	0.000001	-0.000071	-0.000082
15	2.293963	0.000096	0.000100
1	3.008384	1.093756	0.545576
1	3.008379	-1.019147	0.674544
1	3.008508	-0.074383	-1.219731
15	-2.293966	0.000088	0.000085
1	-3.008262	0.074439	1.220069
1	-3.008528	1.019391	-0.674104
1	-3.008480	-1.093535	-0.545350

Adduct Conccis

ΔE_{THF} -3425.61149345
ΔE_{THF} (ZPE) -3425.520034
ΔG_{THF} -3425.568590

15	-1.694991	-2.294834	-0.048916
46	-1.626532	0.000461	-0.027357
15	-1.690990	2.295883	-0.048542
35	3.363642	-0.000682	-0.256983
1	-2.938967	-2.954695	-0.189796
1	-1.002694	-3.021768	-1.046816
1	-1.230842	-3.045471	1.058051
1	-1.225775	3.045650	1.058565
1	-0.997405	3.021823	-1.046271
1	-2.933903	2.957725	-0.189505
6	2.092407	-0.001756	1.258953
1	2.286093	-0.901291	1.838623
1	2.286113	0.896949	1.839901
1	1.085666	-0.001445	0.838250

TS Conccis

ΔE_{THF} -3425.57107978
ΔE_{THF}(ZPE) -3425.481915
ΔG_{THF} -3425.524574

15	1.327442	2.259473	0.012230
46	0.512800	0.027465	0.080659
15	1.791975	-1.920254	-0.320439
35	-2.044576	0.011310	-0.369472
1	2.451202	2.627773	-0.770202
1	0.514274	3.350230	-0.392094
1	1.790795	2.860200	1.210306
1	1.466415	-3.183976	0.240948
1	1.876670	-2.374213	-1.660420
1	3.181992	-2.009068	-0.053070
6	-1.124146	-0.854945	1.610357
1	-1.935658	-0.378119	2.144503
1	-1.272653	-1.910512	1.416806
1	-0.148042	-0.600143	2.045416

Product Conccis

ΔE_{THF} -3425.64368932
ΔE_{THF} (ZPE) -3425.551383
ΔG_{THF} -3425.589817

15	0.176529	2.264111	-0.000175
46	0.401486	-0.146539	-0.000452
15	2.663629	-0.292736	0.000860
35	-2.147418	-0.268203	0.000417
1	1.288257	3.138684	-0.002140
1	-0.543051	2.834583	-1.070538
1	-0.540258	2.835749	1.071435
1	3.257418	-0.987072	1.073111
1	3.259102	-0.972789	-1.079669
1	3.446586	0.880059	0.009058
6	0.447448	-2.233938	-0.000770
1	-0.112147	-2.533512	-0.890261
1	1.436569	-2.701312	-0.013959
1	-0.088261	-2.533484	0.903512

Adduct Conctrans

ΔE_{THF} -3425.61149337
ΔE_{THF}(ZPE) -3425.520036
ΔG_{THF} -3425.568591

15	-1.694598	-2.295011	-0.048811
46	-1.626686	0.000324	-0.027272
15	-1.691472	2.295759	-0.048904
35	3.363878	-0.000784	-0.256948
6	2.092454	-0.000147	1.258812
1	2.285905	-0.899129	1.839418
1	2.286189	0.899111	1.838894
1	1.085775	-0.000121	0.837973
1	-1.218626	3.045693	1.054852
1	-2.935346	2.957537	-0.181388
1	-1.004796	3.021518	-1.051518
1	-1.006889	-3.021834	-1.049947
1	-1.224969	-3.045421	1.055999
1	-2.939079	-2.955159	-0.183712

TS Conctrans

ΔE_{THF} -3425.57087899
ΔE_{THF}(ZPE) -3425.482077
ΔG_{THF} -3425.527221

15	-1.500455	-2.163732	-0.138242
46	-0.541780	0.000260	0.032471
15	-1.495866	2.165878	-0.139947
35	2.020864	-0.002290	-0.369735
6	1.089284	0.002683	1.797555
1	1.611887	-0.907987	2.061338
1	1.609615	0.915738	2.057587
1	0.034909	0.001783	2.104485
1	-0.909463	3.294893	0.489994
1	-2.826610	2.474550	0.241600
1	-1.580218	2.750510	-1.428336
1	-1.613470	-2.736527	-1.429739
1	-0.902656	-3.299421	0.468618
1	-2.823234	-2.473646	0.269012

Product Conctrans

ΔE_{THF} -3425.64805802
ΔE_{THF}(ZPE) -3425.555507
ΔE_{THF} -3425.595785

46	-0.572444	0.049326	-0.000049
15	-0.367585	2.366122	0.000136
1	-1.505969	3.199838	-0.000047
1	0.345412	2.928986	1.076579
1	0.345938	2.929213	-1.075839
15	-0.747715	-2.276488	0.000126
1	-0.141688	-2.954166	-1.075613
1	-0.143311	-2.953531	1.077182
1	-2.014263	-2.898151	-0.000637
6	-2.643705	0.166351	-0.000190
1	-3.015524	-0.343928	-0.894655
1	-3.015651	-0.343537	0.894450
1	-2.998783	1.198443	-0.000444
35	2.030514	-0.153565	-0.000043

Adduct $S_N2$trans

ΔE_{THF} -3425.61084720
ΔE_{THF}(ZPE) -3425.519624
ΔG_{THF} -3425.570819

6	1.981524	-0.428945	-0.126830
1	1.606667	0.103505	-0.996783
1	1.888670	-1.505576	-0.244758
1	1.504158	-0.083117	0.786225
35	3.915187	-0.023950	0.023330
15	-2.140823	-2.220139	0.012927
1	-3.440074	-2.753003	-0.162606
1	-1.491828	-3.042591	-0.939306
1	-1.797948	-2.983840	1.154574
46	-1.843554	0.056292	0.002833
15	-1.688510	2.347359	0.001276
1	-1.268887	3.038678	1.163098
1	-0.834170	3.015268	-0.908746
1	-2.843780	3.124877	-0.250657

TS $S_N2$trans

ΔE_{THF} -3425.59369905
ΔE_{THF}(ZPE) -3425.503227
ΔG_{THF} -3425.546830

6	0.960652	-0.079371	0.001458
1	0.940545	0.474813	-0.923393
1	0.973454	-1.154940	-0.023386
1	0.941972	0.433786	0.949771
35	3.414638	-0.053446	-0.000129
15	-1.787406	-2.280043	0.000972
1	-2.994422	-2.783142	-0.532737
1	-0.895695	-3.134647	-0.685606
1	-1.810747	-2.974878	1.230892
46	-1.473179	0.025283	-0.001326
15	-1.540910	2.358113	0.001217
1	-1.079067	3.078222	1.125656
1	-0.857879	3.095108	-0.992039
1	-2.803419	2.978495	-0.125238

Product $S_N2$trans

ΔE_{THF} -3425.60811344
ΔE_{THF}(ZPE) -3425.516055
ΔG_{THF} -3425.559416

6	0.337306	-0.113623	0.001797
1	0.677878	0.392483	-0.901487
1	0.653265	-1.154738	0.001291
1	0.675781	0.391097	0.906659
35	3.852200	-0.081108	-0.000185
15	-1.867658	-2.293006	0.000096
1	-3.155448	-2.865478	-0.003171
1	-1.279310	-2.982946	-1.076646
1	-1.285256	-2.981946	1.080705
46	-1.712823	0.042051	-0.000352
15	-1.474080	2.401632	0.000138
1	-0.787049	2.989498	1.079010
1	-0.785010	2.989987	-1.077171
1	-2.649773	3.178805	-0.000822

2.1.2.3 $P(CH_3)_3$

$Pd(P(CH_3)_3)_2$

ΔE_{THF} -1050.23487134
ΔE_{THF} (ZPE) -1050.006731
ΔG_{THF} -1050.050565

46	0.000003	-0.000405	0.000183
15	-2.315944	0.000043	0.000090
15	2.315933	-0.000056	-0.000237
6	3.153951	0.534428	1.565326
1	2.847795	-0.120354	2.386233
1	4.244873	0.498343	1.464022
1	2.849873	1.555701	1.812070
6	3.154586	1.088871	-1.245207
1	2.848807	2.127028	-1.086941
1	4.245510	1.018556	-1.163497
1	2.850270	0.793386	-2.253388
6	3.154694	-1.622756	-0.319897
1	2.852780	-2.003840	-1.299637
1	4.245503	-1.517117	-0.295319
1	2.846956	-2.348617	0.438218
6	-3.154110	-0.552083	-1.559230
1	-4.245026	-0.513349	-1.458815
1	-2.846776	0.092302	-2.387876
1	-2.851282	-1.576676	-1.793407
6	-3.155729	-1.073503	1.257582
1	-4.246579	-1.003218	1.174856
1	-2.850804	-2.113717	1.111638
1	-2.851373	-0.766348	2.262262
6	-3.153384	1.627026	0.300723
1	-2.844674	2.343930	-0.465481
1	-4.244259	1.521990	0.276846
1	-2.851600	2.018940	1.276212

Product Conccis

ΔE_{THF} -3661.60476565
ΔE_{THF}(ZPE) -3661.336675
ΔG_{THF} -3661.385721

15	0.958214	1.727807	0.011903
46	-0.105597	-0.480313	0.043868
15	-2.349243	-0.011084	-0.024788
35	2.292921	-1.444158	-0.054303
6	-0.738799	-2.477842	0.145517
1	-0.090808	-2.944289	0.891376
1	-1.781387	-2.658771	0.416136
1	-0.538873	-2.917428	-0.837256
6	2.157793	1.921085	1.404737
1	2.853648	1.080130	1.399628
1	2.710578	2.861764	1.309430
1	1.613581	1.920124	2.353946
6	2.001449	2.004403	-1.487531
1	2.568485	2.937292	-1.400381
1	2.689353	1.164004	-1.602027
1	1.360730	2.055508	-2.372807
6	0.059713	3.344659	0.122865
1	-0.608073	3.475491	-0.731186
1	-0.530174	3.387285	1.042457
1	0.782158	4.167673	0.132488
6	-3.274627	-0.442992	1.511610
1	-4.343971	-0.251368	1.375223
1	-3.126502	-1.494392	1.765414
1	-2.903210	0.168996	2.338117
6	-2.919190	1.718053	-0.321024
1	-2.595492	2.373284	0.489259
1	-2.514309	2.090787	-1.264870
1	-4.012686	1.734049	-0.373637
6	-3.249481	-0.904302	-1.364715
1	-3.103372	-1.981839	-1.276258
1	-4.319415	-0.678293	-1.314017
1	-2.860753	-0.579329	-2.333839

Adduct Conctrans

ΔE_{THF} -3661.56559387
ΔE_{THF}(ZPE) -3661.299444
ΔG_{THF} -3661.355727

15	-1.259759	-2.278805	-0.029260
46	-1.088922	0.033061	0.014269
15	-1.107235	2.351304	-0.025068
35	3.726279	-0.097302	-0.271466
6	2.537905	-0.131246	1.310335
1	2.736541	-1.059863	1.840675
1	2.789367	0.735092	1.917550
1	1.509928	-0.083306	0.941694
6	-0.306040	-3.170795	-1.345372
1	0.762547	-2.975370	-1.220014
1	-0.482237	-4.251856	-1.298728
1	-0.607592	-2.800148	-2.329187
6	-0.758901	-3.228273	1.482957
1	-0.911808	-4.304562	1.342795
1	0.296673	-3.043355	1.700735
1	-1.349621	-2.891143	2.339538
6	-2.967786	-2.942295	-0.312635
1	-3.631781	-2.596111	0.484390
1	-3.351715	-2.566318	-1.265244
1	-2.968546	-4.038275	-0.331144
6	-0.652810	3.162657	-1.628914
1	-0.715832	4.254453	-1.554078
1	0.366714	2.879728	-1.906518
1	-1.329234	2.817042	-2.415859
6	-2.744343	3.146520	0.331002
1	-2.673963	4.239206	0.281143
1	-3.483992	2.801221	-0.396912
1	-3.084598	2.854089	1.328582
6	-0.003069	3.253911	1.160525
1	-0.124098	4.339387	1.068101
1	-0.240959	2.951965	2.184597
1	1.040019	2.992533	0.960376

TS Conctrans

ΔE_{THF} -3661.52167734
ΔE_{THF} (ZPE) -3661.257743
ΔG_{THF} -3661.311383

15	-2.287210	-0.871571	0.049584
46	-0.020921	-0.173333	-0.117199
15	2.212202	-0.986215	0.036439
35	0.130899	2.444686	0.387780
6	-0.030307	1.577655	-1.790539
1	-0.956317	2.101770	-1.991141
1	0.862175	2.111342	-2.092136
1	-0.037234	0.530065	-2.121655
6	-2.950858	-0.935930	1.781216
1	-2.847169	0.047689	2.248024
1	-4.006788	-1.230314	1.792452
1	-2.371667	-1.654974	2.367647
6	-3.575307	0.183622	-0.773627
1	-4.586973	-0.195709	-0.588522
1	-3.502501	1.207121	-0.393732
1	-3.397172	0.206629	-1.853296
6	-2.781239	-2.551024	-0.570944
1	-2.568840	-2.622483	-1.641930
1	-2.191274	-3.315006	-0.056105
1	-3.847544	-2.745670	-0.403889
6	3.015585	-0.714352	1.687615
1	4.056375	-1.058645	1.689001
1	2.988927	0.351231	1.933155
1	2.458494	-1.255238	2.458124
6	2.583501	-2.785618	-0.235923
1	3.651157	-3.001350	-0.108983
1	2.009064	-3.386724	0.475062
1	2.278923	-3.072343	-1.246941
6	3.467182	-0.209163	-1.091181
1	4.474480	-0.598269	-0.902730
1	3.198765	-0.408684	-2.133164
1	3.469830	0.874557	-0.940438

Product Conctrans

ΔE_{THF} -3661.61409654
ΔE_{THF}(ZPE) -3661.346855
ΔG_{THF} -3661.396731

46	0.000606	-0.455855	-0.006070
15	-2.361306	-0.433118	0.002956
15	2.363150	-0.405650	-0.000159
6	0.073327	-2.524190	-0.008246
1	0.630372	-2.856302	-0.890550
1	0.600837	-2.856627	0.892483
1	-0.915763	-2.981170	-0.024398
35	-0.019681	2.179550	-0.001573
6	-3.073393	0.405269	-1.477347
1	-4.164399	0.462328	-1.402243
1	-2.655161	1.411591	-1.551359
1	-2.803384	-0.153536	-2.377808
6	-3.079802	0.503587	1.419708
1	-2.648524	1.506582	1.438118
1	-4.168827	0.569563	1.325200
1	-2.829506	-0.002348	2.356398
6	-3.317869	-2.011000	0.058755
1	-3.060727	-2.578221	0.957566
1	-4.390296	-1.791584	0.071848
1	-3.092703	-2.624963	-0.817415
6	3.092329	0.561633	-1.389620
1	2.657237	1.563199	-1.391575
1	4.180074	0.629323	-1.283182
1	2.852786	0.074227	-2.338856
6	3.054080	0.403375	1.505622
1	4.145535	0.467424	1.444420
1	2.630221	1.405976	1.597202
1	2.776529	-0.176387	2.390386
6	3.313007	-1.985347	-0.078434
1	3.075103	-2.521797	-1.000772
1	4.387033	-1.775385	-0.055439
1	3.056787	-2.625259	0.769680

Adduct $S_N2$trans

ΔE_{THF} -3661.56573820
ΔE_{THF}(ZPE) -3661.299494
ΔG_{THF} -3661.358066

6	-1.856265	-1.917632	0.954515
1	-2.174254	-1.716261	1.974877
1	-1.525359	-2.946768	0.835845
1	-1.098893	-1.205695	0.617870
35	-3.443007	-1.681384	-0.205093
15	2.571126	-1.159498	-0.051895
46	0.995253	0.538270	0.031429
15	-0.459431	2.344661	0.012286
6	-1.707775	2.479288	1.376830
1	-2.325533	3.377115	1.259890
1	-2.354328	1.597369	1.370098
1	-1.193050	2.520675	2.341061
6	-1.540959	2.517975	-1.483487
1	-2.182114	1.636635	-1.573972
1	-2.168011	3.414569	-1.416988
1	-0.917349	2.581165	-2.379751
6	0.330406	4.020479	0.085543
1	1.014932	4.140300	-0.758965
1	-0.423940	4.815228	0.053160
1	0.908554	4.111957	1.009459
6	4.171391	-0.724347	-0.881427
1	4.862312	-1.575507	-0.883842
1	3.976585	-0.416857	-1.912745
1	4.637550	0.114858	-0.357322
6	3.180831	-1.851820	1.556925
1	3.939411	-2.625263	1.391147
1	3.613347	-1.048593	2.160274
1	2.344127	-2.284052	2.113247
6	2.106847	-2.710138	-0.956931

1	2.933489	-3.430030	-0.963709
1	1.237569	-3.168488	-0.476973
1	1.836248	-2.464628	-1.987797

TS $S_N2$trans

ΔE_{THF} -3661.55361350
ΔE_{THF}(ZPE) -3661.288106
ΔG_{THF} -3661.341690

6	1.508996	-0.383207	0.038647
1	1.465764	-0.005286	-0.970426
1	1.268277	-1.415151	0.226694
1	1.558937	0.300895	0.869494
35	3.843104	-0.771781	-0.006049
15	-1.701048	-2.026984	-0.002147
46	-0.969360	0.190265	0.009201
15	-0.615655	2.508360	-0.002744
6	0.442078	3.208058	-1.350203
1	0.500811	4.299502	-1.276943
1	1.451532	2.792739	-1.280487
1	0.024277	2.934907	-2.323229
6	0.143727	3.265711	1.506027
1	1.145973	2.856468	1.662383
1	0.216787	4.354110	1.404091
1	-0.465543	3.026667	2.382064
6	-2.171352	3.494400	-0.182607
1	-2.848990	3.263206	0.643984
1	-1.957409	4.568998	-0.182496
1	-2.667837	3.227232	-1.119587
6	-3.531883	-2.195192	-0.212867
1	-3.833998	-3.248452	-0.206022
1	-4.044115	-1.669436	0.597705
1	-3.833016	-1.741638	-1.161301
6	-1.060376	-3.142102	-1.333079
1	-1.495313	-4.143957	-1.248127
1	-1.310250	-2.723497	-2.312012
1	0.028230	-3.219983	-1.262389
6	-1.395176	-3.034459	1.520193
1	-1.807437	-4.043785	1.412901
1	-0.320169	-3.107886	1.708136
1	-1.860145	-2.545382	2.380736

Product $S_N2$trans

ΔE_{THF} -3661.58048989
ΔE_{THF}(ZPE) -3661.313417
ΔG_{THF} -3661.368006

6	0.709048	-0.125480	-0.116925
1	0.923455	-0.272695	-1.178571
1	1.022103	-0.990330	0.468417
1	1.210789	0.766197	0.256619
35	4.816750	-0.269500	0.011273
15	-1.570014	-2.276687	0.006058
46	-1.320368	0.080517	0.006696
15	-1.109673	2.438043	0.003693
6	-0.168053	3.170726	-1.396698
1	-0.134412	4.261067	-1.307089
1	0.853511	2.782278	-1.401644
1	-0.648210	2.899786	-2.340600
6	-0.330844	3.172771	1.501008
1	0.694729	2.809394	1.604962
1	-0.316805	4.264762	1.426737
1	-0.895909	2.877885	2.389185
6	-2.756670	3.263016	-0.085103
1	-3.368225	2.961443	0.769789
1	-2.641383	4.351696	-0.074453
1	-3.269328	2.966843	-1.004350
6	-3.338962	-2.777594	-0.134058
1	-3.429044	-3.868656	-0.131764
1	-3.907079	-2.371494	0.707389
1	-3.760643	-2.386424	-1.063909
6	-0.743856	-3.176331	-1.369920
1	-0.929548	-4.251919	-1.289524
1	-1.127608	-2.813776	-2.327155
1	0.333792	-2.996859	-1.335676
6	-0.983515	-3.147384	1.518467
1	-1.165484	-4.223607	1.435269
1	0.087934	-2.977813	1.652933
1	-1.509534	-2.757747	2.394000

2.1.2.4 PPh_3

$Pd(PPh_3)_2$

ΔE_{THF} -2200.58424967
ΔE_{THF}(ZPE) -2200.033624
ΔG_{THF} -2200.109274

46	-0.000257	0.003052	0.001513
15	-2.316837	0.000783	-0.000489
15	2.317466	0.000109	0.000016
6	-3.096161	-0.084725	1.675883
6	-2.459228	0.597664	2.726888
6	-4.275897	-0.794975	1.947032
6	-2.998701	0.584693	4.013848
1	-1.532383	1.131771	2.530849
6	-4.808410	-0.817921	3.239453
1	-4.779532	-1.336225	1.151729
6	-4.173994	-0.126451	4.273574
1	-2.495436	1.119374	4.814902
1	-5.720115	-1.376156	3.435102
1	-4.588977	-0.146241	5.277600
6	-3.097951	1.493883	-0.765798
6	-4.281212	2.079942	-0.289739
6	-2.459753	2.065239	-1.880557
6	-4.814427	3.210311	-0.916311
1	-4.786625	1.659486	0.574620
6	-2.999551	3.186286	-2.512409
1	-1.529852	1.632306	-2.242431
6	-4.177915	3.763112	-2.029580
1	-5.728357	3.656190	-0.532908
1	-2.494233	3.615522	-3.373360
1	-4.593399	4.642234	-2.514530
6	-3.093330	-1.410664	-0.910783
6	-2.454472	-2.660879	-0.841352
6	-4.272256	-1.294200	-1.663267
6	-2.990868	-3.771284	-1.494637
1	-1.527350	-2.754868	-0.280058
6	-4.802237	-2.404668	-2.327036
1	-4.777451	-0.335920	-1.737928
6	-4.165706	-3.644621	-2.241774
1	-2.485843	-4.731291	-1.429591
1	-5.713252	-2.297815	-2.909885
1	-4.578479	-4.506230	-2.759343
6	3.095568	1.629904	-0.404474
6	2.458654	2.791103	0.067494
6	4.272291	1.763034	-1.157885
6	2.994854	4.052910	-0.192455
1	1.533109	2.699739	0.631621
6	4.801851	3.028586	-1.427935
1	4.776577	0.880426	-1.539976
6	4.167716	4.174419	-0.943469
1	2.491269	4.940397	0.181264
1	5.711329	3.115855	-2.016403
1	4.580348	5.156959	-1.155597
6	3.097224	-0.463733	1.612889
6	2.461147	-1.451254	2.385273
6	4.276779	0.120066	2.099477
6	3.002151	-1.858233	3.605539
1	1.533196	-1.891734	2.027555
6	4.811531	-0.279992	3.327763
1	4.780540	0.889651	1.522525
6	4.178564	-1.270870	4.080914
1	2.499925	-2.624940	4.189339
1	5.724310	0.183413	3.692692
1	4.595269	-1.579917	5.035640
6	3.095003	-1.165601	-1.208531
6	4.284330	-1.866117	-0.953831
6	2.448687	-1.353795	-2.442645
6	4.816609	-2.731472	-1.914104
1	4.795237	-1.742436	-0.003662
6	2.986865	-2.209392	-3.404813
1	1.514659	-0.832494	-2.639233
6	4.172130	-2.902184	-3.141276
1	5.735768	-3.270693	-1.700953
1	2.475761	-2.342743	-4.354467
1	4.587073	-3.576127	-3.885821

Adduct Conccis

ΔE_{THF} -4811.91629653
ΔE_{THF}(ZPE) -4811.327661
ΔG_{THF} -4811.416335

6	-1.348456	3.429162	-1.290896
1	-2.302980	2.918954	-1.374776
1	-1.109181	3.989979	-2.189845
1	-0.547908	2.744824	-1.023104
15	-2.092011	-0.934462	0.035950
46	0.199368	-0.590796	0.034366
15	2.497861	-0.276724	0.014191
35	-1.516378	4.739880	0.180591
6	-3.023182	-0.023846	-1.280633
6	-2.461817	0.010119	-2.569174
6	-4.233083	0.648328	-1.052889
6	-3.103066	0.686250	-3.607942
1	-1.511931	-0.487116	-2.751880
6	-4.869495	1.336696	-2.091650
1	-4.681513	0.641117	-0.064577
6	-4.308880	1.354914	-3.370322
1	-2.658140	0.699080	-4.599191
1	-5.804679	1.854890	-1.898262
1	-4.805064	1.887554	-4.176692
6	-2.944341	-0.433440	1.598816
6	-4.056894	-1.107405	2.125931
6	-2.438376	0.681335	2.288646
6	-4.651821	-0.672121	3.313497
1	-4.458800	-1.977219	1.615324
6	-3.040135	1.121648	3.468654
1	-1.563098	1.196632	1.900817
6	-4.147919	0.443693	3.985001
1	-5.509470	-1.207005	3.712255
1	-2.637369	1.986449	3.988301
1	-4.612080	0.779723	4.908160
6	-2.622919	-2.689248	-0.215193
6	-1.797474	-3.704326	0.298427
6	-3.800400	-3.050505	-0.889301
6	-2.149124	-5.047571	0.156006
1	-0.871787	-3.433804	0.801142
6	-4.145437	-4.396438	-1.041868
1	-4.447326	-2.282244	-1.302599
6	-3.323128	-5.396517	-0.517541
1	-1.500832	-5.820758	0.559612
1	-5.057798	-4.661335	-1.569472
1	-3.591981	-6.442354	-0.638512
6	3.433198	-1.572295	-0.917406
6	2.792653	-2.182878	-2.009325
6	4.735758	-1.976574	-0.584401
6	3.444104	-3.163328	-2.759800
1	1.774582	-1.891638	-2.258219
6	5.383167	-2.965292	-1.330207
1	5.246313	-1.524889	0.260816
6	4.740674	-3.558293	-2.419668
1	2.935474	-3.625133	-3.601684
1	6.389619	-3.271644	-1.057836
1	5.244953	-4.329097	-2.996005
6	3.313013	-0.256934	1.674863
6	4.453201	0.508792	1.965959
6	2.758218	-1.058362	2.687306
6	5.026442	0.469849	3.239886
1	4.893847	1.141459	1.201258
6	3.337970	-1.104302	3.956249
1	1.862473	-1.637716	2.476659
6	4.472503	-0.337618	4.235761
1	5.906537	1.071147	3.451765
1	2.897358	-1.729354	4.728090
1	4.918931	-0.364869	5.225999
6	3.059018	1.314380	-0.745970
6	2.449956	2.502107	-0.300748
6	4.029147	1.391550	-1.755704
6	2.815779	3.735739	-0.839470
1	1.682800	2.457687	0.468900
6	4.384861	2.628320	-2.305283
1	4.511645	0.488791	-2.117482
6	3.783237	3.801413	-1.848341
1	2.341216	4.643780	-0.477121
1	5.136291	2.669436	-3.089244
1	4.062769	4.761266	-2.273897

TS Conccis

ΔE_{THF} -4811.87340331
ΔE_{THF}(ZPE) -4811.286568
ΔG_{THF} -4811.369584

6	-0.432155	-2.530006	-1.914079
1	0.193856	-3.264320	-2.404991
1	-1.475736	-2.809591	-1.834988
1	-0.247951	-1.520009	-2.299539
15	2.133156	0.217694	-0.034325
46	-0.027420	-0.806053	-0.250847
15	-2.199669	0.122911	-0.031154
35	0.361948	-3.370911	0.125662
6	2.223614	2.044617	0.271524
6	1.248914	2.861544	-0.326959
6	3.206054	2.647809	1.073347
6	1.265453	4.245717	-0.143259
1	0.467355	2.409771	-0.932217
6	3.212358	4.031728	1.270205
1	3.967243	2.039139	1.551308
6	2.245591	4.834263	0.660368
1	0.505330	4.860251	-0.618096
1	3.976092	4.480729	1.899778
1	2.252530	5.909849	0.814420
6	3.194376	-0.482122	1.310501
6	4.587497	-0.625343	1.206144
6	2.561172	-0.891524	2.496462
6	5.328152	-1.160508	2.263594
1	5.097757	-0.322601	0.296495
6	3.302699	-1.417167	3.556499
1	1.480619	-0.809507	2.581646
6	4.688607	-1.554793	3.441267
1	6.405299	-1.267034	2.165771
1	2.796229	-1.729361	4.465915
1	5.265626	-1.972240	4.261901
6	3.179603	-0.006106	-1.548043
6	3.354281	-1.316620	-2.032175
6	3.752192	1.056330	-2.262643
6	4.095077	-1.556379	-3.189274
1	2.906897	-2.151229	-1.497538
6	4.482317	0.815105	-3.431986
1	3.629842	2.076241	-1.912209
6	4.658583	-0.488750	-3.896656
1	4.227715	-2.575771	-3.542141
1	4.917229	1.650911	-3.973795
1	5.229315	-0.674201	-4.802410
6	-3.637422	-0.978825	-0.433060
6	-3.573819	-2.316054	0.001128
6	-4.757594	-0.566206	-1.171839
6	-4.610132	-3.208452	-0.278873
1	-2.704849	-2.660475	0.556779
6	-5.788355	-1.465078	-1.464468
1	-4.831633	0.459026	-1.520415
6	-5.719880	-2.785687	-1.016964
1	-4.545585	-4.235194	0.071326
1	-6.646392	-1.127952	-2.040098
1	-6.522409	-3.482051	-1.243983
6	-2.573147	1.650122	-1.013454
6	-3.382918	2.693065	-0.536288
6	-2.011536	1.766841	-2.296304
6	-3.624206	3.822929	-1.323082
1	-3.823887	2.628245	0.453956
6	-2.262161	2.889787	-3.087356
1	-1.363938	0.978070	-2.671530

6	-3.067296	3.923140	-2.600164
1	-4.249561	4.623338	-0.936577
1	-1.820510	2.961735	-4.077728
1	-3.255410	4.802274	-3.210315
6	-2.552957	0.655690	1.707787
6	-3.733999	0.331966	2.392846
6	-1.570300	1.409865	2.375132
6	-3.926255	0.748395	3.714292
1	-4.506599	-0.248919	1.899397
6	-1.770665	1.837929	3.687729
1	-0.645547	1.661330	1.862243
6	-2.948229	1.503168	4.363892
1	-4.845210	0.484703	4.231165
1	-1.003770	2.425871	4.185102
1	-3.100156	1.827853	5.389610

Product Conccis

ΔE_{THF} -4811.93996358
ΔE_{THF}(ZPE) -4811.350267
ΔG_{THF} -4811.427149

6	-1.496189	-3.066517	0.446112
1	-2.089174	-2.909177	1.351124
1	-2.160204	-3.119390	-0.420354
1	-0.906854	-3.978068	0.532720
46	-0.154857	-1.486562	0.223040
15	-2.016367	-0.103975	-0.006411
15	1.700986	0.232683	0.005221
35	1.704042	-3.248625	0.444592
6	-6.193468	-2.165941	-0.265452
6	-5.569026	-1.726680	-1.433569
6	-4.324829	-1.092393	-1.373250
6	-3.690261	-0.886212	-0.139157
6	-4.325386	-1.336344	1.032120
6	-5.567442	-1.968634	0.968700
1	-7.161424	-2.656577	-0.314278
1	-6.048890	-1.870899	-2.397570
1	-3.859621	-0.753457	-2.292625
1	-3.854545	-1.188944	1.999779
1	-6.045054	-2.305670	1.884403
6	-2.685400	2.685793	3.656458
6	-3.580204	2.728382	2.582791
6	-3.384809	1.905478	1.473177
6	-2.275810	1.041427	1.412884
6	-1.395554	0.993613	2.504248
6	-1.598218	1.811566	3.619556
1	-2.843858	3.322839	4.521962
1	-4.437828	3.394421	2.613010
1	-4.109151	1.926658	0.664626
1	-0.554888	0.306583	2.485227
1	-0.907634	1.759997	4.456446
6	4.038020	0.777449	4.006732
6	4.281008	1.644538	2.937510
6	3.588562	1.487296	1.735990
6	2.647995	0.452775	1.580909
6	2.411806	-0.410393	2.662038
6	3.101673	-0.248053	3.866711
1	4.574789	0.903188	4.943014
1	5.006695	2.446915	3.038510
1	3.777005	2.178333	0.919965
1	1.698805	-1.220714	2.556152
1	2.905636	-0.926505	4.692515
6	4.674761	-1.333217	-3.221755
6	5.174115	-0.901650	-1.991606
6	4.306577	-0.419008	-1.007298
6	2.925553	-0.370534	-1.240663
6	2.430847	-0.819659	-2.476750
6	3.298872	-1.288387	-3.463448
1	5.351134	-1.707890	-3.984974
1	6.241415	-0.941326	-1.791571
1	4.712857	-0.096054	-0.054816
1	1.361343	-0.810071	-2.667032
1	2.899360	-1.629249	-4.414771
6	1.082450	4.724563	-1.146317
6	1.703550	3.862743	-2.050596
6	1.891099	2.514619	-1.728409
6	1.456446	2.007378	-0.494782
6	0.823422	2.883728	0.405095
6	0.641896	4.229098	0.084476
1	0.945073	5.773296	-1.394790
1	2.054523	4.236268	-3.008809
1	2.391021	1.865977	-2.439267
1	0.479595	2.521680	1.368405
1	0.159773	4.890260	0.799594
6	-1.726778	2.199560	-4.038542
6	-1.378927	0.849653	-3.941282
6	-1.450298	0.197716	-2.709182
6	-1.887746	0.881380	-1.560082
6	-2.228286	2.236916	-1.666935
6	-2.143928	2.890333	-2.899395
1	-1.665955	2.710924	-4.995016
1	-1.045594	0.304813	-4.820083
1	-1.163507	-0.848709	-2.637430
1	-2.545918	2.796007	-0.794721
1	-2.402835	3.943341	-2.964287

Adduct Conctrans

ΔE_{THF} -4811.91650658
ΔE_{THF}(ZPE) -4811.327935
ΔG_{THF} -4811.416790

6	-0.949149	3.232361	-1.250254
1	-1.995737	3.141023	-1.527905
1	-0.339828	3.586242	-2.078206
1	-0.562739	2.302471	-0.833590
15	-2.197230	-0.743307	0.020840
46	0.108505	-0.495387	-0.001851
15	2.425164	-0.378589	0.009656
35	-0.844000	4.602891	0.175247
6	-3.090042	0.169520	-1.320083
6	-2.525782	0.147454	-2.608330
6	-4.265358	0.905529	-1.109921
6	-3.130939	0.832176	-3.662820
1	-1.601073	-0.399478	-2.778310
6	-4.863659	1.604006	-2.164303
1	-4.715223	0.941816	-0.122726
6	-4.300931	1.567352	-3.441575
1	-2.684368	0.801658	-4.653043
1	-5.771170	2.173943	-1.984107
1	-4.767316	2.109429	-4.259562
6	-3.026387	-0.169997	1.572287
6	-4.180176	-0.769730	2.101192
6	-2.461342	0.925087	2.248566
6	-4.757293	-0.281126	3.276808
1	-4.628818	-1.622231	1.599965
6	-3.044790	1.418994	3.416616
1	-1.556012	1.384352	1.859055
6	-4.193830	0.814722	3.934522
1	-5.647838	-0.758588	3.676760
1	-2.595983	2.267459	3.926003
1	-4.644026	1.192205	4.848542
6	-2.794786	-2.482957	-0.178810
6	-2.021205	-3.512254	0.384946
6	-3.974600	-2.818949	-0.861340
6	-2.425767	-4.844035	0.281675
1	-1.093586	-3.263208	0.895281
6	-4.372749	-4.154180	-0.973680
1	-4.582764	-2.040066	-1.311657
6	-3.602002	-5.168015	-0.400627
1	-1.817361	-5.628315	0.723946
1	-5.286382	-4.399388	-1.508623
1	-3.912449	-6.205442	-0.489977
6	3.248825	-1.842331	-0.767560
6	2.556505	-2.523503	-1.783067
6	4.521700	-2.300249	-0.391375
6	3.129251	-3.627261	-2.418296
1	1.559807	-2.189017	-2.062132
6	5.089443	-3.411206	-1.020229
1	5.070717	-1.795069	0.397671
6	4.396463	-4.074679	-2.036008
1	2.581309	-4.142689	-3.202461
1	6.073469	-3.757189	-0.715314
1	4.839357	-4.939280	-2.522797
6	3.197992	-0.285035	1.688223
6	4.398074	0.395195	1.949571
6	2.546594	-0.940980	2.746666
6	4.935888	0.413768	3.239378
1	4.912622	0.917943	1.148741
6	3.089667	-0.929645	4.032568
1	1.605184	-1.451890	2.557331
6	4.285199	-0.250018	4.281909
1	5.863768	0.947424	3.427135
1	2.574189	-1.442268	4.840273
1	4.703918	-0.232758	5.284400
6	3.166339	1.068852	-0.876094
6	2.726107	2.355855	-0.516100
6	4.105770	0.942892	-1.909685
6	3.225521	3.486257	-1.162900
1	1.986044	2.474031	0.271804
6	4.594783	2.076863	-2.567795
1	4.459868	-0.039445	-2.205388
6	4.159954	3.349184	-2.195366
1	2.879789	4.472626	-0.865317
1	5.319880	1.960335	-3.368875
1	4.542800	4.228969	-2.705113

TS Conctrans

ΔE_{THF} -4811.87277981
ΔE_{THF}(ZPE) -4811.285964
ΔG_{THF} -4811.368687

6	-0.124077	-2.256491	-2.000804
1	0.710176	-2.822390	-2.395277
1	-1.097047	-2.704857	-2.157949
1	-0.076567	-1.193673	-2.270384
15	2.207858	0.237503	-0.038863
46	-0.018508	-0.637059	-0.206211
15	-2.251206	0.176786	-0.029248
35	0.201674	-3.248058	0.100449
6	3.453535	-0.751689	-0.990083
6	3.307004	-0.834204	-2.387624
6	4.473458	-1.495959	-0.379040
6	4.166975	-1.622794	-3.151855
1	2.516453	-0.274386	-2.882553
6	5.328187	-2.296599	-1.144974
1	4.604568	-1.455778	0.697620
6	5.180596	-2.360837	-2.531062
1	4.043477	-1.664557	-4.230872
1	6.112054	-2.866235	-0.652825
1	5.846995	-2.980485	-3.124636
6	2.881517	0.230556	1.689037
6	3.871152	1.122742	2.133334
6	2.368936	-0.713257	2.595598
6	4.336842	1.069864	3.449516
1	4.279158	1.865558	1.454785
6	2.842801	-0.772140	3.908378
1	1.594440	-1.402196	2.269517
6	3.826051	0.121636	4.339461
1	5.099786	1.770823	3.777761
1	2.436884	-1.511044	4.594225
1	4.189191	0.082545	5.362837
6	2.552228	1.968380	-0.606069
6	1.540392	2.926759	-0.432937
6	3.770883	2.370817	-1.178043
6	1.744821	4.256636	-0.806239
1	0.584075	2.622311	-0.016347
6	3.971057	3.699346	-1.562209
1	4.565684	1.646588	-1.329262
6	2.960656	4.645736	-1.374190
1	0.949244	4.983401	-0.665982
1	4.918660	3.993691	-2.005652
1	3.117937	5.678250	-1.674088
6	-2.581458	1.881233	-0.681487
6	-1.879074	2.293971	-1.826159
6	-3.489460	2.774549	-0.090866
6	-2.091120	3.558669	-2.378217
1	-1.151275	1.623046	-2.276191
6	-3.689683	4.047008	-0.633539

1	-4.040412	2.480949	0.797455
6	-2.995510	4.440409	-1.780083
1	-1.540718	3.859212	-3.265733
1	-4.391195	4.728702	-0.159886
1	-3.153407	5.429545	-2.201197
6	-2.847872	0.271837	1.720959
6	-4.181056	0.043235	2.098182
6	-1.909999	0.595738	2.716378
6	-4.566104	0.140825	3.438158
1	-4.921407	-0.215678	1.347155
6	-2.297747	0.703864	4.053173
1	-0.870945	0.753307	2.437211
6	-3.627291	0.474155	4.417357
1	-5.601168	-0.041814	3.714555
1	-1.560166	0.957788	4.809828
1	-3.928856	0.549458	5.458533
6	-3.565864	-0.835606	-0.857998
6	-3.578297	-2.220430	-0.605130
6	-4.506858	-0.309068	-1.756088
6	-4.517759	-3.049718	-1.218919
1	-2.844713	-2.651234	0.071860
6	-5.439753	-1.144020	-2.380919
1	-4.517530	0.754627	-1.971435
6	-5.450836	-2.513501	-2.112610
1	-4.515951	-4.115234	-1.004952
1	-6.160251	-0.717914	-3.074169
1	-6.177784	-3.159849	-2.596651

Product Conctrans

ΔE_{THF} -4811.94950319
ΔE_{THF}(ZPE) -4811.359758
ΔG_{THF} -4811.436043

6	0.000750	2.150228	0.225407
1	-0.493127	2.559682	-0.661157
1	-0.581115	2.414725	1.112230
1	0.997163	2.586699	0.308135
46	0.013138	0.078801	0.026867
15	2.387093	0.219401	0.032102
15	-2.381076	0.111379	0.017827
35	-0.052768	-2.522174	-0.219674
6	3.368445	-1.266549	-0.452246
6	3.445749	-2.348938	0.441278
6	4.000941	-1.369197	-1.699749
6	4.155546	-3.499388	0.099067
1	2.950238	-2.295758	1.405568
6	4.704678	-2.527577	-2.043143
1	3.955250	-0.547289	-2.406514
6	4.785865	-3.592935	-1.145651
1	4.210919	-4.324985	0.803126
1	5.192574	-2.589838	-3.011974
1	5.336246	-4.490975	-1.412082
6	2.987752	1.535734	-1.116004
6	4.045993	2.403841	-0.811784
6	2.340727	1.660828	-2.357877
6	4.453581	3.371776	-1.734391
1	4.552082	2.336685	0.145349
6	2.757374	2.619836	-3.282389
1	1.501908	1.011534	-2.596111
6	3.814927	3.479154	-2.971104
1	5.270744	4.041819	-1.482002
1	2.250221	2.700835	-4.239793
1	4.134135	4.231849	-3.686449
6	3.063482	0.628358	1.698439
6	4.433092	0.497453	1.991110
6	2.193368	1.063715	2.710562
6	4.919422	0.814339	3.260306
1	5.120996	0.135253	1.233026
6	2.682431	1.378252	3.981159
1	1.130784	1.146038	2.505100
6	4.045412	1.257519	4.257124
1	5.979969	0.709056	3.471022
1	1.995394	1.711455	4.754015
1	4.425437	1.499229	5.245773
6	-3.055187	-0.840963	-1.410224
6	-2.384000	-0.739698	-2.640510
6	-4.200869	-1.644209	-1.325547
6	-2.861825	-1.409959	-3.767229
1	-1.473704	-0.150154	-2.711965
6	-4.669759	-2.325608	-2.452076
1	-4.725675	-1.755326	-0.382672
6	-4.006422	-2.206332	-3.674734
1	-2.331927	-1.320980	-4.711549
1	-5.553787	-2.951834	-2.369344
1	-4.373253	-2.737494	-4.548565
6	-3.149367	-0.582613	1.542842
6	-4.512193	-0.385766	1.831964
6	-2.361279	-1.308106	2.449629
6	-5.073071	-0.915044	2.995052
1	-5.136084	0.190952	1.155859
6	-2.925042	-1.832890	3.615610
1	-1.310614	-1.471752	2.235491
6	-4.280110	-1.639577	3.889488
1	-6.127584	-0.756905	3.203279
1	-2.301908	-2.392754	4.307484
1	-4.717207	-2.047719	4.796582
6	-3.203413	1.762584	-0.127280
6	-3.665708	2.251255	-1.358964
6	-3.296649	2.591286	1.005485
6	-4.216620	3.532374	-1.453952
1	-3.607799	1.632180	-2.248252
6	-3.849338	3.869058	0.908536
1	-2.947657	2.236642	1.971146
6	-4.310657	4.344155	-0.322449
1	-4.576529	3.890051	-2.414713
1	-3.920035	4.491763	1.796076
1	-4.741921	5.338461	-0.396881

Adduct $S_N2$trans

ΔE_{THF} -4811.91620407
ΔE_{THF}(ZPE) -4811.327429
ΔG_{THF} -4811.415679

6	1.635307	3.447291	0.320126
1	0.566610	3.363744	0.140306
1	2.207638	2.822077	-0.359519
1	1.884851	3.245852	1.358769
35	2.142478	5.326124	-0.042372
15	1.971918	-1.222410	-0.005222
46	-0.297514	-0.751614	0.007054
15	-2.544671	-0.187782	0.006001
6	-2.857045	1.636133	0.069047
6	-3.699147	2.246866	1.009193
6	-2.172535	2.447818	-0.854699
6	-3.854827	3.637537	1.025487
1	-4.235722	1.641813	1.733194
6	-2.341588	3.832577	-0.848062
1	-1.501486	1.990455	-1.578088
6	-3.180892	4.432437	0.097919
1	-4.508115	4.094968	1.763686
1	-1.814347	4.443679	-1.575851
1	-3.304937	5.511691	0.109917
6	-3.523175	-0.859430	1.424932
6	-4.896105	-1.143845	1.350983
6	-2.845839	-1.098179	2.632818
6	-5.575387	-1.650106	2.462122
1	-5.437158	-0.977632	0.424218
6	-3.527606	-1.594529	3.745502
1	-1.777408	-0.902800	2.689701
6	-4.894160	-1.873358	3.661305
1	-6.637064	-1.870205	2.388862
1	-2.989410	-1.773437	4.672402
1	-5.424298	-2.268900	4.523361
6	-3.502519	-0.730661	-1.480263
6	-4.563269	0.007842	-2.028625
6	-3.143227	-1.949235	-2.081555
6	-5.251734	-0.465445	-3.149153
1	-4.850620	0.957412	-1.586724
6	-3.838777	-2.426032	-3.193848
1	-2.307131	-2.516455	-1.678778
6	-4.893850	-1.683511	-3.731386
1	-6.068475	0.118800	-3.564577
1	-3.549279	-3.370410	-3.646805
1	-5.429543	-2.049205	-4.603099
6	2.431513	-2.882116	-0.679431
6	1.587071	-3.964596	-0.375976
6	3.564188	-3.109965	-1.476088
6	1.878214	-5.246603	-0.843585
1	0.694659	-3.794455	0.222284
6	3.847317	-4.392688	-1.954978
1	4.226247	-2.287173	-1.728751
6	3.008421	-5.462853	-1.637570
1	1.217343	-6.073442	-0.597706
1	4.725624	-4.552862	-2.574598
1	3.229998	-6.458820	-2.011114
6	2.976808	-0.043653	-1.019439
6	4.245976	0.419814	-0.639853
6	2.415016	0.427795	-2.219427
6	4.937253	1.333643	-1.441751
1	4.696792	0.076071	0.285970
6	3.110905	1.329737	-3.025791
1	1.422353	0.092610	-2.511040
6	4.373698	1.788801	-2.635823
1	5.916780	1.687237	-1.131346
1	2.663603	1.682835	-3.951011
1	4.911604	2.499395	-3.257177
6	2.799112	-1.180851	1.649701
6	3.874775	-2.012166	1.998746
6	2.318525	-0.261127	2.598120
6	4.460004	-1.920037	3.265001
1	4.257132	-2.735728	1.284860
6	2.910996	-0.162073	3.858174
1	1.468935	0.368946	2.344907
6	3.982758	-0.993872	4.194947
1	5.289519	-2.573299	3.522103
1	2.529531	0.556214	4.578947
1	4.438919	-0.924353	5.178630

TS $S_N2$trans

ΔE_{THF} -4811.90205742
ΔE_{THF}(ZPE) -4811.314425
ΔE_{THF} -4811.399847

6	-0.002535	2.329419	0.019640
1	-0.800446	2.267073	-0.701655
1	1.020198	2.312722	-0.314694
1	-0.229651	2.245220	1.070166
35	-0.054515	4.722174	0.072331
15	2.343109	-0.418464	0.010789
46	0.011263	-0.187861	0.049333
15	-2.324926	-0.454155	0.023396
6	-3.319303	0.902868	-0.735860
6	-4.378841	1.542554	-0.076955
6	-2.951366	1.344541	-2.020488
6	-5.060537	2.597299	-0.692675
1	-4.675773	1.222242	0.916524
6	-3.638448	2.390686	-2.635802
1	-2.121923	0.868674	-2.539419
6	-4.694555	3.022037	-1.970530
1	-5.877809	3.085251	-0.168782
1	-3.343681	2.718796	-3.628616
1	-5.224125	3.843086	-2.445332
6	-3.065323	-0.703647	1.696000
6	-4.233455	-1.454353	1.906525
6	-2.426199	-0.117704	2.801347
6	-4.752793	-1.607831	3.193900
1	-4.736392	-1.926304	1.067742
6	-2.951068	-0.265429	4.086852
1	-1.509103	0.446290	2.652023
6	-4.114888	-1.011993	4.285150
1	-5.655504	-2.193915	3.342902
1	-2.446137	0.194932	4.931596
1	-4.520074	-1.134063	5.285780
6	-2.843307	-1.955578	-0.921019
6	-4.040574	-2.023179	-1.651180
6	-2.000028	-3.079491	-0.893953
6	-4.386909	-3.191460	-2.335563
1	-4.702304	-1.163362	-1.692953

6	-2.351904	-4.248038	-1.571172
1	-1.061403	-3.035133	-0.346800
6	-3.545855	-4.305620	-2.295308
1	-5.315455	-3.228456	-2.898676
1	-1.689209	-5.108537	-1.540875
1	-3.816365	-5.212180	-2.829450
6	2.783374	-2.156240	-0.435115
6	2.202186	-3.194471	0.316376
6	3.633867	-2.484400	-1.500609
6	2.477816	-4.528050	0.015765
1	1.532376	-2.956579	1.139610
6	3.899171	-3.823265	-1.807252
1	4.091013	-1.699445	-2.094614
6	3.325357	-4.845933	-1.050740
1	2.027146	-5.318504	0.609672
1	4.558998	-4.062255	-2.636798
1	3.534439	-5.884907	-1.289639
6	3.228244	0.621587	-1.229836
6	4.535314	1.098638	-1.045292
6	2.543390	0.952956	-2.412186
6	5.144507	1.885856	-2.025911
1	5.079147	0.861733	-0.136055
6	3.157192	1.732167	-3.394367
1	1.523085	0.603736	-2.554483
6	4.458942	2.202187	-3.201093
1	6.154998	2.252704	-1.868426
1	2.614704	1.981485	-4.302023
1	4.933958	2.817773	-3.959756
6	3.253114	-0.133789	1.591421
6	4.416379	-0.842282	1.934290
6	2.764472	0.839358	2.478913
6	5.078206	-0.576321	3.135399
1	4.804812	-1.606158	1.267316
6	3.431739	1.109662	3.675070
1	1.855874	1.382325	2.235285
6	4.589267	0.400775	4.005973
1	5.975862	-1.133480	3.389150
1	3.042972	1.867632	4.349333
1	5.105080	0.605319	4.939982

Product $S_N2$trans

ΔE_{THF} -4811.92854546

ΔE_{THF}(ZPE) -4811.339227

ΔG_{THF} -4811.422966

6	0.007312	1.147556	1.592745
1	0.922667	1.040131	2.174358
1	-0.866954	0.963387	2.217071
1	-0.045604	2.126686	1.107897
35	-0.135991	4.910560	0.135339
15	-2.350527	-0.416440	0.026476
46	0.017852	-0.239931	0.085446
15	2.379293	-0.368411	0.034462
6	3.202545	-0.567879	1.663098
6	4.469416	-0.029744	1.934638
6	2.528320	-1.279899	2.670848
6	5.054431	-0.210268	3.190377
1	4.998509	0.533418	1.173063
6	3.120396	-1.465692	3.920640
1	1.536630	-1.681877	2.477100
6	4.384003	-0.928760	4.182369
1	6.033618	0.214677	3.391393
1	2.590698	-2.018420	4.691225
1	4.840584	-1.064240	5.158613
6	3.281994	0.953892	-0.859177
6	4.500532	0.691859	-1.511178
6	2.754673	2.255230	-0.880662
6	5.179534	1.718176	-2.168715
1	4.915194	-0.311832	-1.512448
6	3.440244	3.278031	-1.540076
1	1.812590	2.486779	-0.393009
6	4.650336	3.012173	-2.183688
1	6.119577	1.505851	-2.670177
1	3.017387	4.278237	-1.549313
1	5.179030	3.808809	-2.699544
6	2.735000	-1.906172	-0.913930
6	3.279529	-3.054069	-0.318284
6	2.373869	-1.945584	-2.274161
6	3.465628	-4.216435	-1.071699
1	3.564093	-3.044618	0.728947

6	2.564619	-3.107440	-3.022100
1	1.954874	-1.064228	-2.753500
6	3.109765	-4.246363	-2.421597
1	3.894883	-5.096282	-0.600879
1	2.289711	-3.121657	-4.072881
1	3.258189	-5.150792	-3.004414
6	-2.675642	-2.010081	-0.837007
6	-2.128591	-2.184213	-2.122327
6	-3.396832	-3.061540	-0.252375
6	-2.309836	-3.384249	-2.809868
1	-1.570999	-1.377202	-2.592367
6	-3.572767	-4.263396	-0.944211
1	-3.825090	-2.945286	0.737865
6	-3.031312	-4.427203	-2.220756
1	-1.889070	-3.503810	-3.804111
1	-4.138529	-5.068389	-0.483874
1	-3.171174	-5.361877	-2.756073
6	-3.202640	-0.529924	1.647357
6	-4.460308	0.047858	1.876596
6	-2.559699	-1.214044	2.694308
6	-5.066815	-0.065500	3.130224
1	-4.965695	0.588418	1.082970
6	-3.173104	-1.332728	3.941546
1	-1.575265	-1.647205	2.534230
6	-4.427322	-0.756065	4.161555
1	-6.038705	0.389411	3.298375
1	-2.667185	-1.863913	4.742658
1	-4.900574	-0.839291	5.135698
6	-3.249012	0.842669	-0.960028
6	-4.429014	0.520611	-1.654013
6	-2.755218	2.156326	-1.011516
6	-5.103673	1.500686	-2.383310
1	-4.817320	-0.493366	-1.631372
6	-3.437716	3.132959	-1.740249
1	-1.841116	2.434168	-0.494918
6	-4.609235	2.807724	-2.426807
1	-6.013599	1.242059	-2.917562
1	-3.039976	4.142984	-1.770394
1	-5.134817	3.568251	-2.997492

2.1.3 Species Optimized in DMF

CH_3Br

ΔE_{DMF} -2611.32920214
ΔE_{DMF}(ZPE) -2611.292019
ΔG_{DMF} -2611.315914

6	0.000000	0.000000	-1.550099
35	0.000000	0.000000	0.426228
1	0.000000	1.038299	-1.872463
1	0.899193	-0.519149	-1.872463
1	-0.899193	-0.519149	-1.872463

2.1.3.1 PF_3

$Pd(PF_3)_2$

ΔE_{DMF} -1409.96820182
ΔE_{DMF}(ZPE) -1409.950050
ΔG_{DMF} -1409.992774

46	-0.000005	-0.758205	0.000052
15	-2.033436	0.156726	0.000005
15	2.033449	0.156716	-0.000029
9	3.088203	-0.045749	-1.206136
9	3.087997	-0.045216	1.206345
9	2.095628	1.767407	-0.000386
9	-2.095656	1.767414	-0.000335
9	-3.087972	-0.045241	1.206386
9	-3.088198	-0.045750	-1.206098

Adduct Conccis

ΔE_{DMF} -4021.30756533
ΔE_{DMF}(ZPE) -4021.251391
ΔG_{DMF} -4021.305573

15	2.263344	-0.614438	-0.004688
46	0.118182	-0.007000	0.003824
15	-0.577066	2.115285	-0.001893
35	-1.709700	-1.984670	0.007390
6	-3.516499	-1.159443	-0.029763
1	-4.225631	-1.983719	-0.037883
1	-3.603347	-0.552996	0.867468
1	-3.569965	-0.563872	-0.936875
9	2.931591	-1.420107	1.226410
9	2.909773	-1.507968	-1.187111
9	3.389202	0.542606	-0.058221
9	0.508963	3.287642	-0.238907
9	-1.239374	2.776479	1.314149
9	-1.654944	2.691348	-1.061873

TS Conccis

ΔE_{DMF} -4021.26084917
ΔE_{DMF}(ZPE) -4021.206235
ΔG_{DMF} -4021.256216

15	-1.384536	1.693751	0.029361
46	0.013567	-0.169292	0.163478
15	2.246333	0.257548	-0.101034
35	-1.326645	-2.236848	-0.418422
6	0.078903	-2.059881	1.589193
1	-0.764099	-2.543851	2.060699
1	0.870269	-2.720098	1.257631
1	0.400499	-1.163815	2.131189
9	-2.981225	1.583216	-0.155244
9	-1.411072	2.702150	1.282689
9	-1.148098	2.803046	-1.111280
9	2.879895	1.662314	0.366539
9	2.772988	0.315037	-1.619405
9	3.432119	-0.666357	0.482838

Product Conccis

ΔE_{DMF} -4021.30689869
ΔE_{DMF}(ZPE) -4021.249852
ΔG_{DMF} -4021.297130

15	0.898044	1.689953	0.000032
46	-0.099561	-0.481009	0.000298
15	-2.271960	-0.026048	0.000086
35	2.275956	-1.344344	-0.000428
6	-0.713136	-2.489595	0.000496
1	-0.253931	-2.891725	0.903480
1	-1.788374	-2.667335	0.002829
1	-0.257899	-2.890800	-0.904932
9	1.865436	2.057681	1.206746
9	1.864115	2.057850	-1.207703
9	0.017480	3.019962	0.000602
9	-3.159361	-0.554672	1.203918
9	-3.159349	-0.556791	-1.202815
9	-2.749535	1.487894	-0.001286

Adduct Conctrans

ΔE_{DMF} -4021.30754660
ΔE_{DMF}(ZPE) -4021.251356
ΔG_{DMF} -4021.304282

15	2.254437	-0.635088	-0.008212
46	0.113480	-0.005468	0.003266
15	-0.557255	2.122824	-0.003819
35	-1.720128	-1.976186	-0.000737
6	-3.525328	-1.146729	-0.008791
1	-4.236726	-1.968924	-0.009973
1	-3.597623	-0.543969	0.892177
1	-3.590940	-0.547198	-0.912409
9	-1.543078	2.726819	-1.134397
9	0.555444	3.285881	-0.135793
9	-1.313270	2.771914	1.268754
9	2.849790	-1.880802	-0.852764
9	3.361480	0.426067	-0.514802
9	2.990073	-0.991825	1.384447

TS Conctrans

ΔE_{DMF} -4021.26074153
ΔE_{DMF}(ZPE) -4021.206304
ΔG_{DMF} -4021.256353

15	2.053154	-1.010445	-0.055053
46	0.000037	0.053544	-0.020385
15	-2.053016	-1.010714	-0.055033
35	-0.000282	2.554106	-0.353334
6	0.000143	1.470288	1.876425
1	0.916580	2.000077	2.097582
1	-0.916383	1.999828	2.097809
1	0.000322	0.422410	2.190791
9	-2.205934	-2.519071	-0.598338
9	-3.294976	-0.406908	-0.885006
9	-2.834376	-1.229156	1.334091
9	2.206212	-2.518718	-0.598556
9	3.295023	-0.406419	-0.884996
9	2.834577	-1.228995	1.334021

Product Conctrans

ΔE_{DMF} -4021.30553273
ΔE_{DMF}(ZPE) -4021.248503
ΔE_{DMF} -4021.297009

46	0.003141	-0.426628	-0.093259
15	-2.278147	-0.426616	0.048596
15	2.288787	-0.393270	0.049068
6	0.061464	-2.516589	-0.188852
1	0.727005	-2.775759	-1.014445
1	0.453644	-2.880534	0.763078
1	-0.933013	-2.919125	-0.370120
35	-0.032692	2.159570	-0.043138
9	-3.122166	-1.771703	0.025791
9	-3.091668	0.381884	-1.044342
9	-2.895249	0.220351	1.356444
9	3.093571	0.431623	-1.037899
9	2.900190	0.249509	1.361586
9	3.140178	-1.732424	0.015019

Adduct $S_N2$trans

ΔE_{DMF} -4021.29870640
ΔE_{DMF}(ZPE) -4021.242396
ΔG_{DMF} -4021.298425

6	-2.732974	-1.361138	-0.061287
1	-2.215317	-1.123745	0.865344
1	-2.910344	-2.429087	-0.159840
1	-2.208985	-0.959654	-0.925706
35	-4.500730	-0.478213	0.011659
15	2.251888	-1.615487	-0.001123
46	0.675040	-0.042814	0.003587
15	0.832474	2.177449	-0.004244
9	2.322148	2.788907	-0.065185
9	0.333394	3.088732	1.231870
9	0.229578	3.106769	-1.179386
9	2.632876	-2.414467	1.348021
9	3.750364	-1.125364	-0.334965
9	2.280613	-2.893821	-0.989760

TS $S_N2$trans

ΔE_{DMF} -4021.26316158
ΔE_{DMF}(ZPE) -4021.207854
ΔG_{DMF} -4021.257617

6	1.254215	-0.062838	-0.163140
1	1.304594	0.121347	0.901291
1	1.475258	0.750674	-0.842626
1	1.431017	-1.069233	-0.514696
35	3.940613	-0.092164	0.048088
15	-1.119528	2.251441	0.106706
9	-2.525533	2.713114	0.698603
9	-0.179616	2.797163	1.272778
9	-0.910825	3.453648	-0.924013
46	-0.955162	0.015884	-0.481909
15	-1.260529	-2.178100	0.114975
9	-0.045534	-3.211896	0.109554
9	-1.792459	-2.472974	1.588949
9	-2.325959	-3.060250	-0.679829

Product $S_N2$trans

ΔE_{DMF} -4021.26424140
ΔE_{DMF}(ZPE) -4021.208187
ΔG_{DMF} -4021.259843

6	1.004402	-0.017651	-0.144915
1	1.177639	0.166659	0.911822
1	1.341814	0.779329	-0.803330
1	1.315100	-1.002034	-0.479125
35	4.105491	-0.078336	0.026465
15	-1.136119	2.289647	0.100398
9	-2.485725	2.793644	0.765565
9	-0.098960	2.838199	1.168257
9	-0.968967	3.424530	-0.999456
46	-1.082762	0.020564	-0.420053
15	-1.250767	-2.243062	0.101815
9	0.021209	-3.190063	0.034464
9	-1.730892	-2.584771	1.575643
9	-2.285868	-3.141651	-0.699684

2.1.3.2 PH_3

$Pd(PH_3)_2$

ΔE_{DMF} -814.281936931
ΔE_{DMF}(ZPE) -814.228229
ΔG_{DMF} -814.259870

46	0.000009	-0.000034	0.000081
15	2.294516	0.000076	-0.000005
1	3.005557	-0.965333	-0.751751
1	3.006142	1.133291	-0.460765
1	3.007813	-0.168201	1.210761
15	-2.294563	0.000134	0.000083
1	-3.004276	-0.663416	-1.028973
1	-3.007740	-0.559132	1.087015
1	-3.007222	1.221190	-0.061180

Adduct Conccis

ΔE_{DMF} -3425.61265437
ΔE_{DMF}(ZPE) -3425.521273
ΔG_{DMF} -3425.570569

15	-1.663211	-2.296648	-0.049782
46	-1.599565	0.000016	-0.026320
15	-1.663078	2.296680	-0.049779
35	3.294684	-0.000030	-0.270163
1	-2.889818	-2.959513	-0.289834
1	-0.888627	-3.023162	-0.985025
1	-1.288234	-3.038407	1.095654
1	-1.288255	3.038402	1.095732
1	-0.888263	3.023138	-0.984874
1	-2.889586	2.959647	-0.290055
6	2.097179	-0.000028	1.306116
1	2.318702	-0.899602	1.875405
1	2.318733	0.899525	1.875426
1	1.072648	-0.000007	0.930711

TS Conccis

ΔE_{DMF} -3425.57227281
ΔE_{DMF}(ZPE) -3425.483075
ΔG_{DMF} -3425.525577

15	1.357178	2.249334	0.018439
46	0.514642	0.026808	0.072531
15	1.771252	-1.939223	-0.316856
35	-2.050791	0.028837	-0.364584
1	2.493101	2.604941	-0.751522
1	0.565346	3.356829	-0.382745
1	1.818814	2.829425	1.226723
1	1.424258	-3.190745	0.257170
1	1.860280	-2.407724	-1.651407
1	3.157681	-2.038864	-0.037637
6	-1.128892	-0.858092	1.608277
1	-1.942142	-0.386932	2.144571
1	-1.273036	-1.912284	1.404750
1	-0.153232	-0.600182	2.040706

Product Conccis

ΔE_{DMF} -3425.64735877
ΔE_{DMF}(ZPE) -3425.554821
ΔG_{DMF} -3425.594491

15	0.211364	2.265368	-0.000233
46	0.400378	-0.149273	-0.000491
15	2.662235	-0.309665	0.000898
35	-2.161258	-0.255425	0.000450
1	1.339364	3.116502	-0.001551
1	-0.498532	2.848497	-1.070406
1	-0.495987	2.848513	1.071626
1	3.245688	-1.004719	1.077476
1	3.247291	-0.998971	-1.078535
1	3.447593	0.860191	0.004550
6	0.438650	-2.236412	-0.000741
1	-0.113668	-2.535422	-0.895606
1	1.424875	-2.709544	-0.005136
1	-0.105826	-2.535693	0.898880

Adduct Conctrans

ΔE_{DMF} -3425.61265437
ΔE_{DMF}(ZPE) -3425.521273
ΔG_{DMF} -3425.570559

15	-1.663144	-2.296651	-0.049764
46	-1.599639	0.000013	-0.026329
15	-1.663013	2.296684	-0.049776
35	3.294692	-0.000032	-0.270165
6	2.097195	-0.000008	1.306126
1	2.318781	-0.899536	1.875462
1	2.318709	0.899590	1.875379
1	1.072661	-0.000063	0.930727
1	-1.286598	3.038362	1.095244
1	-2.889748	2.959810	-0.288449
1	-0.889326	3.023043	-0.985881
1	-0.888989	-3.022970	-0.985515
1	-1.287353	-3.038420	1.095400
1	-2.889776	-2.959722	-0.289118

TS Conctrans

ΔE_{DMF} -3425.57204424
ΔE_{DMF}(ZPE) -3425.483209
ΔG_{DMF} -3425.527179

15	-1.503118	-2.163923	-0.134074
46	-0.542573	0.000000	0.025805
15	-1.503078	2.163942	-0.134099
35	2.028410	-0.000026	-0.367647
6	1.092933	0.000050	1.800336
1	1.613427	-0.912490	2.061245
1	1.613415	0.912616	2.061180
1	0.037250	0.000050	2.100261
1	-0.831294	3.324824	0.330407
1	-2.759217	2.494636	0.433729
1	-1.791729	2.672337	-1.424931
1	-1.792082	-2.672203	-1.424879
1	-0.831277	-3.324871	0.330187
1	-2.759143	-2.494616	0.434008

Product Conctrans

ΔE_{DMF} -3425.65086462
ΔE_{DMF}(ZPE) -3425.558285
ΔG_{DMF} -3425.598477

46	-0.572687	0.044725	-0.000075
15	-0.402250	2.367145	-0.000030
1	-1.553111	3.182048	0.000183
1	0.303181	2.940099	1.076143
1	0.302861	2.940212	-1.076354
15	-0.738291	-2.285006	-0.000038
1	-0.130015	-2.959695	-1.076384
1	-0.130637	-2.959503	1.076781
1	-2.003091	-2.908313	-0.000334
6	-2.643689	0.140496	0.000257
1	-3.008131	-0.374289	-0.894498
1	-3.007890	-0.374287	0.895112
1	-3.008147	1.169055	0.000308
35	2.044253	-0.136792	0.000057

Adduct $S_N2$trans

ΔE_{DMF} -3425.61197184
ΔE_{DMF}(ZPE) -3425.520790
ΔG_{DMF} -3425.571947

6	-1.980009	-0.315096	0.031163
1	-1.586077	0.182716	0.913025
1	-1.840126	-1.391801	0.080783
1	-1.565264	0.102638	-0.882215
35	-3.934695	0.017173	-0.005660
15	2.005686	-2.263507	-0.002389
1	3.280217	-2.877816	-0.003855
1	1.451498	-3.020393	1.057172
1	1.449439	-3.019479	-1.061523
46	1.856632	0.027989	-0.001192
15	1.828900	2.324748	-0.000142
1	1.219385	3.035137	-1.061583
1	1.210838	3.034147	1.057009
1	3.050591	3.038259	0.005118

TS $S_N2$trans

ΔE_{DMF} -3425.59680781
ΔE_{DMF}(ZPE) -3425.506368
ΔG_{DMF} -3425.549794

6	1.004287	-0.077786	0.002152
1	0.950149	0.467924	-0.926389
1	0.983760	-1.153542	-0.012643
1	0.952540	0.443665	0.944660
35	3.419629	-0.051983	-0.000242
15	-1.787341	-2.279487	0.000923
1	-2.998266	-2.780963	-0.525304
1	-0.901816	-3.135052	-0.692473
1	-1.803426	-2.976541	1.229745
46	-1.481103	0.024972	-0.001338
15	-1.546402	2.354721	0.001179
1	-1.063975	3.077324	1.115434
1	-0.883355	3.092006	-1.005456
1	-2.811461	2.974090	-0.101967

Product $S_N2$trans

ΔE_{DMF} -3425.62142281
ΔE_{DMF}(ZPE) -3425.529807
ΔG_{DMF} -3425.571634

6	-0.059345	-0.337941	0.003268
1	-0.474973	0.109338	0.908151
1	-0.216872	-1.416135	0.003482
1	-0.479597	0.109633	-0.899346
35	-4.461994	-0.190606	-0.000304
15	2.462594	-2.165531	0.001968
1	3.832678	-2.491849	-0.003573
1	2.014008	-2.941849	1.086779
1	2.003164	-2.949625	-1.072725
46	1.932250	0.118385	-0.002299
15	1.359261	2.411980	0.002247
1	0.594664	2.906228	-1.071336
1	0.610099	2.905110	1.087049
1	2.431370	3.325564	-0.004918

2.1.3.3 $P(CH_3)_3$

$Pd(P(CH_3)_3)_2$

ΔE_{DMF} -1050.23649656
ΔE_{DMF}(ZPE) -1050.008165
ΔG_{DMF} -1050.054062

46	-0.000005	0.000320	0.000071
15	2.318821	0.000008	-0.000107
15	-2.318831	-0.000212	0.000268
6	-3.151012	1.654224	0.078945
1	-2.843988	2.259232	-0.778982
1	-4.241845	1.548654	0.072435
1	-2.846504	2.174073	0.991775
6	-3.153877	-0.895240	1.392092
1	-2.851849	-0.452234	2.345453
1	-4.244561	-0.839905	1.299556
1	-2.846419	-1.944893	1.388793
6	-3.152286	-0.758086	-1.471779
1	-2.849164	-1.804906	-1.564566
1	-4.243104	-0.706803	-1.378574
1	-2.844744	-0.230365	-2.379081
6	3.150501	-1.654236	-0.087707
1	4.241354	-1.548925	-0.081236
1	2.843791	-2.263456	0.767365
1	2.845347	-2.169449	-1.002940
6	3.153346	0.902178	-1.387605
1	4.244075	0.845630	-1.296322
1	2.850191	0.464697	-2.343170
1	2.846495	1.951965	-1.378126
6	3.153374	0.749898	1.475467
1	2.846014	0.217746	2.380234
1	4.244120	0.698461	1.381443
1	2.850909	1.796415	1.573799

Product Conccis

ΔE_{DMF} -3661.60861415
ΔE_{DMF}(ZPE) -3661.340643
ΔG_{DMF} -3661.389962

15	0.933570	1.740130	0.012002
46	-0.101571	-0.482355	0.044113
15	-2.348848	-0.028415	-0.028057
35	2.315839	-1.432538	-0.059105
6	-0.723745	-2.482774	0.160192
1	-0.049835	-2.949406	0.883049
1	-1.755611	-2.667059	0.466695
1	-0.558791	-2.923193	-0.829211
6	2.121831	1.942632	1.413618
1	2.832698	1.114190	1.408668
1	2.659396	2.892851	1.327637
1	1.571063	1.927844	2.358872
6	1.984085	2.031576	-1.479817
1	2.534560	2.973791	-1.388150
1	2.687861	1.203787	-1.590051
1	1.348647	2.073188	-2.369359
6	0.016266	3.344869	0.119921
1	-0.644011	3.470912	-0.740422
1	-0.581904	3.377885	1.034299
1	0.731284	4.174047	0.138574
6	-3.255574	-0.425896	1.527620
1	-4.325198	-0.230736	1.400221
1	-3.110474	-1.473287	1.799530
1	-2.870608	0.201451	2.336153
6	-2.925596	1.688531	-0.369176
1	-2.616372	2.364326	0.429405
1	-2.514332	2.041558	-1.317668
1	-4.018534	1.692271	-0.432905
6	-3.248714	-0.962115	-1.339621
1	-3.098394	-2.036358	-1.224258
1	-4.319060	-0.738932	-1.288969
1	-2.866608	-0.658634	-2.318223

Adduct Conctrans

ΔE_{DMF} -3661.56766280
ΔE_{DMF}(ZPE) -3661.301398
ΔG_{DMF} -3661.359506

15	-2.420623	-1.303563	-0.049122
46	-0.994853	0.527769	0.001892
15	0.320158	2.441181	0.004258
35	3.384292	-1.662076	-0.244978
6	1.989661	-1.678343	1.161340
1	1.685590	-2.713662	1.295834
1	2.442023	-1.273672	2.063663
1	1.166242	-1.055344	0.804521
6	-2.173311	-2.520832	-1.424902
1	-1.165801	-2.942301	-1.366667
1	-2.906734	-3.333275	-1.368482
1	-2.276637	-2.010742	-2.386900
6	-2.423830	-2.419368	1.430945
1	-3.135194	-3.243366	1.303753
1	-1.422209	-2.831766	1.581951
1	-2.696300	-1.845149	2.321147
6	-4.226962	-0.925368	-0.220992
1	-4.553990	-0.308669	0.621013
1	-4.398068	-0.364784	-1.144389
1	-4.820996	-1.846110	-0.244084
6	1.464942	2.671650	-1.435157
1	2.028718	3.607137	-1.344798
1	2.165651	1.833368	-1.483134
1	0.886392	2.689565	-2.363212
6	-0.595909	4.052414	0.003246
1	0.098195	4.900480	-0.002112
1	-1.237512	4.108563	-0.880721
1	-1.230201	4.113744	0.892173
6	1.476549	2.682596	1.432677
1	2.036598	3.619296	1.332777
1	0.906268	2.703615	2.365799
1	2.181119	1.847583	1.479085

TS Conctrans

ΔE_{DMF} -3661.52357460
ΔE_{DMF}(ZPE) -3661.259638
ΔG_{DMF} -3661.313397

15	-2.286418	-0.878001	0.049984
46	-0.017717	-0.182468	-0.112550
15	2.224855	-0.972425	0.037804
35	0.110274	2.447088	0.385364
6	-0.032106	1.565763	-1.795811
1	-0.959793	2.085188	-1.999873
1	0.861114	2.101426	-2.090902
1	-0.033545	0.516461	-2.119775
6	-2.960317	-0.931903	1.777787
1	-2.859999	0.054257	2.240206
1	-4.016416	-1.225174	1.782460
1	-2.386721	-1.649093	2.371999
6	-3.564754	0.174523	-0.789515
1	-4.577621	-0.204327	-0.611149
1	-3.495385	1.199633	-0.413372
1	-3.376325	0.192368	-1.867369
6	-2.773099	-2.561237	-0.564235
1	-2.551990	-2.638925	-1.632977
1	-2.188621	-3.322193	-0.038640
1	-3.840770	-2.753882	-0.404913
6	2.996032	-0.787351	1.715665
1	4.039680	-1.122203	1.714796
1	2.956436	0.262366	2.020779
1	2.431893	-1.376873	2.444285
6	2.616601	-2.749641	-0.330622
1	3.684169	-2.961127	-0.197095
1	2.036744	-3.396250	0.334593
1	2.333878	-2.979774	-1.362237
6	3.486923	-0.120067	-1.024072
1	4.493204	-0.517174	-0.848215
1	3.230421	-0.255448	-2.079166
1	3.482787	0.952059	-0.805848

Product Conctrans

ΔE_{DMF} -3661.61679379
ΔE_{DMF}(ZPE) -3661.349660
ΔG_{DMF} -3661.399846

46	0.000835	-0.452685	-0.006219
15	-2.364542	-0.439649	0.002418
15	2.366878	-0.411052	-0.000026
6	0.074714	-2.519534	-0.007107
1	0.633256	-2.850351	-0.888732
1	0.602086	-2.848980	0.894583
1	-0.914450	-2.975636	-0.023800
35	-0.020985	2.193021	-0.001308
6	-3.081318	0.402537	-1.473656
1	-4.172149	0.456005	-1.395121
1	-2.667483	1.410794	-1.546347
1	-2.812799	-0.153503	-2.376256
6	-3.084053	0.488193	1.424682
1	-2.660529	1.494486	1.445994
1	-4.173615	0.547115	1.333456
1	-2.828363	-0.020278	2.358516
6	-3.313559	-2.021233	0.052228
1	-3.057264	-2.588369	0.951241
1	-4.386478	-1.804910	0.062175
1	-3.083501	-2.632077	-0.824738
6	3.097520	0.549285	-1.393749
1	2.671363	1.554735	-1.396536
1	4.185944	0.608686	-1.290734
1	2.851902	0.061232	-2.341075
6	3.061974	0.400194	1.502785
1	4.153448	0.459433	1.439275
1	2.643665	1.405281	1.593058
1	2.784139	-0.176907	2.389174
6	3.309309	-1.994361	-0.074510
1	3.070819	-2.530594	-0.996728
1	4.383659	-1.787085	-0.050231
1	3.049862	-2.631297	0.774733

Adduct $S_N2$trans

ΔE_{DMF} -3661.56765171
ΔE_{DMF}(ZPE) -3661.301425
ΔG_{DMF} -3661.359449

6	-1.957907	-1.767113	1.153765
1	-2.407557	-1.420653	2.081622
1	-1.656089	-2.809910	1.220206
1	-1.134164	-1.124698	0.835143
35	-3.354927	-1.656329	-0.246037
15	2.397027	-1.308463	-0.052416
46	0.984229	0.532654	0.006362
15	-0.317467	2.455317	0.008380
6	-1.582291	2.638473	1.350957
1	-2.122867	3.587006	1.255594
1	-2.296946	1.812491	1.296746
1	-1.089204	2.603466	2.326659
6	-1.344670	2.765565	-1.502655
1	-2.043779	1.936821	-1.645510
1	-1.908725	3.700681	-1.410301
1	-0.695785	2.823050	-2.381198
6	0.604194	4.056321	0.158636
1	1.313597	4.149621	-0.668572
1	-0.082885	4.909988	0.140709
1	1.166856	4.068243	1.096460
6	4.075266	-1.018900	-0.783814
1	4.673575	-1.936886	-0.768107
1	3.970309	-0.676163	-1.817110
1	4.594454	-0.242305	-0.215123
6	2.838326	-2.085233	1.571897
1	3.517695	-2.933992	1.432737

1	3.319945	-1.341955	2.213730
1	1.929552	-2.432427	2.071684
6	1.830694	-2.784127	-1.020347
1	2.581782	-3.581847	-0.996554
1	0.893403	-3.160822	-0.601326
1	1.649656	-2.492980	-2.058962

TS $S_N2$trans

ΔE_{DMF} -3661.55627036
ΔE_{DMF}(ZPE) -3661.291025
ΔG_{DMF} -3661.345807

6	1.547188	-0.381121	0.040489
1	1.479361	-0.004279	-0.967990
1	1.291589	-1.409045	0.233312
1	1.574114	0.310246	0.866871
35	3.858515	-0.753674	-0.006413
15	-1.696679	-2.034408	-0.002083
46	-0.972143	0.185563	0.008787
15	-0.631662	2.505006	-0.002634
6	0.443146	3.210115	-1.333712
1	0.491118	4.302106	-1.261777
1	1.454554	2.803197	-1.245443
1	0.043746	2.931514	-2.312887
6	0.096053	3.270496	1.517647
1	1.097939	2.867823	1.692182
1	0.163334	4.359060	1.414088
1	-0.527423	3.029711	2.383203
6	-2.192104	3.477572	-0.210807
1	-2.881056	3.242768	0.605309
1	-1.986424	4.553691	-0.209582
1	-2.670662	3.204513	-1.155384
6	-3.525967	-2.202148	-0.225271
1	-3.827904	-3.255356	-0.215366
1	-4.043706	-1.672496	0.579226
1	-3.819622	-1.753442	-1.178354
6	-1.047873	-3.154555	-1.325095
1	-1.486455	-4.154732	-1.239782
1	-1.290296	-2.738591	-2.307049
1	0.039933	-3.235273	-1.245551
6	-1.402053	-3.036597	1.525938
1	-1.811921	-4.046667	1.417118
1	-0.328546	-3.107427	1.723104
1	-1.876352	-2.546138	2.380613

Product $S_N2$trans

ΔE_{DMF} -3661.59350403
ΔE_{DMF}(ZPE) -3661.327381
ΔG_{DMF} -3661.383888

6	0.669213	-0.000611	-0.261865
1	0.819685	-0.000795	-1.345407
1	1.106581	-0.892276	0.189311
1	1.107454	0.890773	0.189063
35	5.090412	-0.001176	0.022947
15	-1.418591	-2.363466	0.010547
46	-1.350115	0.000348	0.014337
15	-1.416456	2.364209	0.010493
6	-0.560219	3.216115	-1.377754
1	-0.674001	4.301104	-1.289122
1	0.503925	2.966271	-1.367024
1	-0.987162	2.883891	-2.327578
6	-0.746280	3.185480	1.515606
1	0.314524	2.945425	1.626224
1	-0.862004	4.271599	1.444250
1	-1.279429	2.821616	2.397880
6	-3.152669	2.973009	-0.096046
1	-3.731538	2.588535	0.748025
1	-3.174846	4.067360	-0.078105
1	-3.609012	2.619390	-1.024452
6	-3.155230	-2.971135	-0.095351
1	-3.178075	-4.065465	-0.076914
1	-3.733691	-2.585922	0.748656
1	-3.611525	-2.617662	-1.023833
6	-0.563605	-3.215765	-1.378257
1	-0.677619	-4.300718	-1.289492
1	-0.991170	-2.883465	-2.327773
1	0.500619	-2.966221	-1.368358
6	-0.748368	-3.185474	1.515240
1	-0.865085	-4.271479	1.443777
1	0.312702	-2.946375	1.625386
1	-1.280780	-2.821271	2.397819

2.1.3.4 PPh_3

$Pd(PPh_3)_2$

ΔE_{DMF} -2200.58753550
ΔE_{DMF}(ZPE) -2200.036875
ΔG_{DMF} -2200.112101

46	-0.001025	0.002307	-0.004667
15	2.318047	0.000354	-0.000912
15	-2.320798	0.000267	-0.001241
6	3.093972	-0.921134	-1.404858
6	2.462678	-0.855449	-2.659625
6	4.268816	-1.678381	-1.277358
6	3.001883	-1.518115	-3.763179
1	1.540475	-0.288061	-2.764441
6	4.801360	-2.351523	-2.380982
1	4.770068	-1.747526	-0.316784
6	4.172132	-2.270562	-3.625038
1	2.503372	-1.455530	-4.726633
1	5.709474	-2.937091	-2.265912
1	4.587336	-2.795103	-4.481112
6	3.094136	1.677131	-0.094989
6	4.273355	1.945161	-0.807484
6	2.458301	2.731242	0.584465
6	4.805630	3.237723	-0.836293
1	4.778157	1.147918	-1.344677
6	2.997188	4.018447	0.564773
1	1.532824	2.538653	1.122777
6	4.171673	4.274993	-0.148980
1	5.717251	3.430669	-1.395315
1	2.495002	4.821770	1.096909
1	4.586675	5.278769	-0.173195
6	3.091451	-0.755835	1.500236
6	2.445394	-1.859537	2.084384
6	4.280472	-0.283847	2.077848
6	2.983182	-2.485057	3.210169
1	1.513034	-2.220653	1.655802
6	4.811972	-0.904110	3.212447
1	4.793689	0.569822	1.645643
6	4.167165	-2.005921	3.778682
1	2.473098	-3.338441	3.648596
1	5.731219	-0.525224	3.650891
1	4.581486	-2.485908	4.660921
6	-3.097792	1.595458	-0.524842
6	-2.454883	2.335616	-1.532577
6	-4.283694	2.098624	0.032441
6	-2.993179	3.541885	-1.983264
1	-1.524284	1.964349	-1.956312
6	-4.815430	3.313043	-0.411489
1	-4.793922	1.546985	0.816302
6	-4.174303	4.034807	-1.420671
1	-2.485416	4.100847	-2.764549
1	-5.732135	3.692065	0.032129
1	-4.589129	4.978629	-1.763476
6	-3.095673	-1.253490	-1.119298
6	-2.455684	-2.498758	-1.249066
6	-4.277307	-1.021397	-1.840186
6	-2.992446	-3.492938	-2.068257
1	-1.528765	-2.681257	-0.709763
6	-4.807518	-2.013961	-2.669915
1	-4.785642	-0.065521	-1.758110
6	-4.169163	-3.250842	-2.783479
1	-2.487129	-4.450853	-2.156135
1	-5.721065	-1.818485	-3.224908
1	-4.582623	-4.020390	-3.429428
6	-3.091454	-0.343424	1.644948
6	-4.262489	-1.099772	1.809028
6	-2.458779	0.182293	2.785268
6	-4.789358	-1.322007	3.084952
1	-4.764998	-1.520769	0.943439
6	-2.992177	-0.030500	4.057154
1	-1.539584	0.752666	2.670764
6	-4.158435	-0.786273	4.209775
1	-5.694473	-1.912835	3.196631
1	-2.492205	0.384272	4.928170
1	-4.569376	-0.960728	5.200276

Adduct Conccis

ΔE_{DMF} -4811.91964558
ΔE_{DMF}(ZPE) -4811.331122
ΔG_{DMF} -4811.420735

6	-1.335673	3.421071	-1.356644
1	-2.320659	3.105048	-1.688761
1	-0.821622	4.008814	-2.113097
1	-0.735845	2.576715	-1.024604
15	-2.087161	-0.923669	0.021814
46	0.206216	-0.571688	-0.002364
15	2.505261	-0.250427	0.002194
35	-1.601411	4.599696	0.212194
6	-3.029806	0.006614	-1.271579
6	-2.495864	0.036171	-2.572547
6	-4.221947	0.699615	-1.014581
6	-3.147232	0.727801	-3.594503
1	-1.560525	-0.478751	-2.780281
6	-4.867369	1.405119	-2.036276
1	-4.650629	0.695396	-0.017424
6	-4.334792	1.418661	-3.327193
1	-2.724392	0.736114	-4.595396
1	-5.788566	1.939384	-1.820328
1	-4.838358	1.964519	-4.120087
6	-2.916176	-0.449896	1.606048
6	-4.035239	-1.121186	2.123604
6	-2.386436	0.637310	2.323083
6	-4.612375	-0.711360	3.329064
1	-4.457068	-1.967814	1.590449
6	-2.969987	1.052148	3.521630
1	-1.508500	1.152397	1.940309
6	-4.083727	0.376078	4.028452
1	-5.475710	-1.243337	3.719409
1	-2.548723	1.894618	4.063433
1	-4.533385	0.692001	4.965664
6	-2.614261	-2.676371	-0.247885
6	-1.784608	-3.696795	0.248494
6	-3.794692	-3.030442	-0.920672
6	-2.133813	-5.038808	0.088273
1	-0.857510	-3.432940	0.752539
6	-4.138012	-4.374906	-1.089387
1	-4.446532	-2.258636	-1.319019
6	-3.310850	-5.380518	-0.583928
1	-1.482474	-5.816060	0.478537
1	-5.052984	-4.633899	-1.615199
1	-3.578737	-6.424910	-0.717560
6	3.449279	-1.512584	-0.965889
6	2.824306	-2.077814	-2.091021
6	4.746037	-1.932377	-0.629351
6	3.485059	-3.030211	-2.869151
1	1.811405	-1.773842	-2.345985
6	5.402566	-2.893387	-1.403102
1	5.245304	-1.514800	0.239765
6	4.775399	-3.442009	-2.524417
1	2.988629	-3.457154	-3.736283
1	6.404594	-3.211479	-1.128297
1	5.287155	-4.190304	-3.123215
6	3.295186	-0.298285	1.674496
6	4.411237	0.478325	2.024277
6	2.742792	-1.162772	2.635433
6	4.964013	0.387517	3.305004
1	4.850122	1.158433	1.300412
6	3.302296	-1.260528	3.910513
1	1.864803	-1.751964	2.380350
6	4.413510	-0.482831	4.248676
1	5.826078	0.996887	3.562426
1	2.864643	-1.934905	4.641520
1	4.844262	-0.550964	5.243758
6	3.075985	1.366517	-0.693516
6	2.403825	2.530347	-0.277648
6	4.122682	1.486438	-1.619652
6	2.781280	3.782978	-0.762895
1	1.578451	2.452369	0.426374
6	4.490191	2.741487	-2.117006
1	4.655298	0.602901	-1.957176
6	3.824428	3.890939	-1.688993
1	2.256414	4.672354	-0.424671
1	5.301056	2.816385	-2.836482
1	4.112667	4.864842	-2.074526

TS Conccis

ΔE_{DMF} -4811.87627211
ΔE_{DMF}(ZPE) -4811.289583
ΔG_{DMF} -4811.373467

6	-0.439154	-2.528333	-1.914394
1	0.188071	-3.261849	-2.404710
1	-1.482927	-2.806674	-1.835606
1	-0.253003	-1.516504	-2.292925
15	2.138480	0.211968	-0.033930
46	-0.028838	-0.804269	-0.243159
15	-2.203151	0.126899	-0.031090
35	0.345761	-3.377777	0.128409
6	2.228177	2.041689	0.252894
6	1.274957	2.855297	-0.384063
6	3.188675	2.650324	1.076763
6	1.290899	4.241248	-0.215127
1	0.511474	2.399831	-1.009382
6	3.193730	4.036587	1.258948
1	3.934700	2.044975	1.581960
6	2.248463	4.835435	0.611813
1	0.548808	4.853601	-0.720295
1	3.940243	4.490028	1.905601
1	2.254700	5.912554	0.754011
6	3.192579	-0.475043	1.323452
6	4.584740	-0.629845	1.221855
6	2.556165	-0.862882	2.515198
6	5.320979	-1.156470	2.286916
1	5.097998	-0.341032	0.309422
6	3.293118	-1.379787	3.582834
1	1.476412	-0.769100	2.600065
6	4.678120	-1.530085	3.469642
1	6.397340	-1.271600	2.191321
1	2.784463	-1.674137	4.496932
1	5.251767	-1.940182	4.296190
6	3.191732	-0.028082	-1.540618
6	3.321875	-1.336333	-2.044355
6	3.819904	1.021917	-2.226771
6	4.072810	-1.587054	-3.192856
1	2.830878	-2.161098	-1.533229
6	4.560063	0.770681	-3.387672
1	3.733564	2.040066	-1.860957
6	4.691258	-0.531564	-3.871962
1	4.169366	-2.604748	-3.561743
1	5.037692	1.596901	-3.907579
1	5.269259	-0.724907	-4.771334
6	-3.641918	-0.973931	-0.430965
6	-3.579257	-2.312188	-0.000056
6	-4.764591	-0.557269	-1.163831
6	-4.618388	-3.202254	-0.277778
1	-2.708936	-2.659735	0.551520
6	-5.798321	-1.453510	-1.454237
1	-4.838641	0.468991	-1.509251
6	-5.730347	-2.775539	-1.010326
1	-4.554663	-4.229941	0.069683
1	-6.658225	-1.113353	-2.025100
1	-6.535103	-3.469748	-1.235628
6	-2.568877	1.649621	-1.022155
6	-3.375425	2.697894	-0.550948
6	-2.006426	1.756872	-2.305633
6	-3.612032	3.824561	-1.343916
1	-3.818519	2.639895	0.438767
6	-2.252408	2.876751	-3.102644
1	-1.363155	0.963148	-2.677867

6	-3.053732	3.915919	-2.621157
1	-4.235094	4.628975	-0.962300
1	-1.810401	2.941693	-4.093258
1	-3.238150	4.792485	-3.235949
6	-2.557674	0.668350	1.705328
6	-3.732472	0.333994	2.396242
6	-1.582190	1.438104	2.366027
6	-3.925169	0.754312	3.716613
1	-4.500612	-0.257274	1.908303
6	-1.783039	1.869987	3.677415
1	-0.662407	1.699999	1.849212
6	-2.954130	1.523896	4.359477
1	-4.839405	0.482648	4.237529
1	-1.022117	2.470181	4.169191
1	-3.106553	1.851840	5.383973

Product Conccis

ΔE_{DMF} -4811.94412256
ΔE_{DMF} (ZPE) -4811.354374
ΔG_{DMF} -4811.431260

6	-1.503390	-3.052894	0.468650
1	-2.108080	-2.882282	1.364136
1	-2.157792	-3.120486	-0.404481
1	-0.916648	-3.964549	0.577430
46	-0.156499	-1.480724	0.231696
15	-2.017659	-0.100107	-0.007174
15	1.700035	0.236825	0.001917
35	1.707100	-3.255572	0.469285
6	-6.193327	-2.167265	-0.244246
6	-5.559829	-1.756829	-1.418274
6	-4.315671	-1.121751	-1.364164
6	-3.690292	-0.885905	-0.130470
6	-4.334020	-1.307484	1.046814
6	-5.576165	-1.940744	0.989499
1	-7.161641	-2.657517	-0.288340
1	-6.032925	-1.923646	-2.381892
1	-3.843874	-0.805339	-2.288203
1	-3.870768	-1.136701	2.014219
1	-6.061133	-2.254474	1.909554
6	-2.669331	2.716590	3.636955
6	-3.566825	2.753572	2.565253
6	-3.376896	1.921790	1.461263
6	-2.270117	1.054399	1.404834
6	-1.387076	1.012259	2.494275
6	-1.584531	1.839061	3.603951
1	-2.823511	3.360974	4.497671
1	-4.422103	3.422577	2.592146
1	-4.103530	1.940040	0.654818
1	-0.547774	0.323623	2.478113
1	-0.891733	1.792368	4.439233
6	4.029456	0.792317	4.006180
6	4.303348	1.630657	2.921415
6	3.613722	1.469027	1.718802
6	2.646116	0.457543	1.577587
6	2.377924	-0.375593	2.674918
6	3.064467	-0.208471	3.881024
1	4.563171	0.922365	4.943481
1	5.050299	2.414442	3.011427
1	3.825983	2.139020	0.891093
1	1.637769	-1.163378	2.583680
1	2.841886	-0.861574	4.720394
6	4.659037	-1.364970	-3.222942
6	5.163489	-0.934012	-1.994379
6	4.301159	-0.439580	-1.010912
6	2.920111	-0.379007	-1.242973
6	2.420477	-0.825771	-2.478382
6	3.283342	-1.306397	-3.464274
1	5.331331	-1.747251	-3.985874
1	6.230693	-0.981268	-1.795769
1	4.712370	-0.114539	-0.061245
1	1.351414	-0.803051	-2.670143
1	2.880051	-1.642901	-4.415481
6	1.104860	4.726204	-1.168006
6	1.725568	3.858610	-2.067294
6	1.906414	2.510734	-1.739649
6	1.464726	2.010068	-0.505641
6	0.833639	2.892318	0.389901
6	0.658836	4.237351	0.063611
1	0.971746	5.774256	-1.421091
1	2.081018	4.227196	-3.025679
1	2.405456	1.857788	-2.447140
1	0.484931	2.535512	1.353411
1	0.177100	4.903242	0.774416
6	-1.740940	2.168050	-4.059700
6	-1.384279	0.821171	-3.951096
6	-1.450252	0.179510	-2.713136
6	-1.890269	0.870836	-1.569573
6	-2.240011	2.223376	-1.687679
6	-2.161444	2.866375	-2.926114
1	-1.684791	2.671211	-5.020710
1	-1.048576	0.270752	-4.825378
1	-1.157126	-0.864477	-2.633060
1	-2.562076	2.788061	-0.820826
1	-2.428495	3.916684	-3.000170

Adduct Conctrans

ΔE_{DMF} -4811.91964516
ΔE_{DMF} (ZPE) -4811.331128
ΔG_{DMF} -4811.420797

6	-1.332716	3.420300	-1.357163
1	-2.316461	3.104875	-1.693516
1	-0.815659	4.009002	-2.110816
1	-0.734335	2.575337	-1.024031
15	-2.086925	-0.923486	0.021933
46	0.206394	-0.571286	-0.001922
15	2.505441	-0.249943	0.002368
35	-1.604204	4.596755	0.212292
6	-3.029477	0.007749	-1.270843
6	-2.496269	0.036892	-2.572126
6	-4.220712	0.702018	-1.013058
6	-3.147475	0.729356	-3.593617
1	-1.561622	-0.479023	-2.780511
6	-4.865931	1.408377	-2.034292
1	-4.648821	0.698105	-0.015659
6	-4.334106	1.421500	-3.325523
1	-2.725201	0.737336	-4.594750
1	-5.786411	1.943636	-1.817744
1	-4.837536	1.968031	-4.118039
6	-2.916166	-0.451149	1.606473
6	-4.036041	-1.122252	2.122530
6	-2.385914	0.634640	2.325259
6	-4.613460	-0.713640	3.328256
1	-4.458268	-1.967805	1.587983
6	-2.969736	1.048272	3.524100
1	-1.507387	1.149560	1.943613
6	-4.084276	0.372401	4.029416
1	-5.477422	-1.245457	3.717427
1	-2.548073	1.889650	4.067287
1	-4.534151	0.687390	4.966839
6	-2.613868	-2.676024	-0.249192
6	-1.784919	-3.696729	0.247819
6	-3.793436	-3.029719	-0.923659
6	-2.134008	-5.038638	0.086561
1	-0.858461	-3.433184	0.753203
6	-4.136621	-4.374094	-1.093424
1	-4.444697	-2.257689	-1.322512
6	-3.310194	-5.379980	-0.587334
1	-1.483235	-5.816108	0.477338
1	-5.050926	-4.632785	-1.620544
1	-3.577967	-6.424296	-0.721774
6	3.449405	-1.511359	-0.966718
6	2.824026	-2.076420	-2.091709
6	4.746531	-1.930732	-0.631077
6	3.484736	-3.028244	-2.870580
1	1.810850	-1.772770	-2.345970
6	5.403026	-2.891160	-1.405576
1	5.246110	-1.513286	0.237923
6	4.775449	-3.439617	-2.526744
1	2.987992	-3.455072	-3.737588
1	6.405345	-3.208934	-1.131465
1	5.287184	-4.187461	-3.126124
6	3.295805	-0.298734	1.674439
6	4.411858	0.477799	2.024394
6	2.743807	-1.163906	2.634984
6	4.965007	0.386261	3.304905
1	4.850435	1.158436	1.300840
6	3.303681	-1.262384	3.909849
1	1.865838	-1.753078	2.379779
6	4.414884	-0.484751	4.248187
1	5.827066	0.995582	3.562465
1	2.866322	-1.937279	4.640554
1	4.845926	-0.553451	5.243105
6	3.075780	1.367533	-0.692441
6	2.404348	2.531120	-0.274735
6	4.121399	1.488074	-1.619712
6	2.781480	3.784112	-0.759300
1	1.579801	2.452686	0.430206
6	4.488576	2.743497	-2.116369
1	4.653440	0.604738	-1.958659
6	3.823562	3.892700	-1.686531
1	2.257215	4.673292	-0.419634
1	5.298607	2.818881	-2.836733
1	4.111556	4.866892	-2.071515

TS Conctrans

ΔE_{DMF} -4811.87569445
ΔE_{DMF}(ZPE) -4811.288915
ΔG_{DMF} -4811.371658

6	-0.173670	-2.368916	-1.909514
1	0.642170	-2.952816	-2.316681
1	-1.154543	-2.813398	-2.023808
1	-0.121717	-1.314266	-2.203915
15	2.187904	0.220835	-0.031228
46	-0.025687	-0.707159	-0.139499
15	-2.240307	0.161250	-0.018631
35	0.224244	-3.306136	0.208385
6	3.390599	-0.679675	-1.113290
6	3.149014	-0.704534	-2.500203
6	4.469520	-1.421800	-0.608710
6	3.974662	-1.432268	-3.357398
1	2.311538	-0.147709	-2.914655
6	5.289456	-2.161931	-1.467983
1	4.676216	-1.426012	0.456751
6	5.047979	-2.167501	-2.842489
1	3.777541	-1.428759	-4.426101
1	6.120216	-2.729867	-1.057716
1	5.687826	-2.739523	-3.508525
6	2.977833	0.152584	1.644056
6	4.045939	0.986297	2.016702
6	2.484059	-0.770485	2.580887
6	4.606797	0.895216	3.292563
1	4.440176	1.712177	1.311587
6	3.050083	-0.865609	3.855198
1	1.652204	-1.414914	2.309839
6	4.111131	-0.031482	4.214329
1	5.430861	1.548855	3.565697
1	2.656266	-1.586188	4.567034
1	4.547510	-0.099619	5.207017
6	2.441249	1.993939	-0.509163
6	1.468516	2.922620	-0.100793
6	3.552628	2.457195	-1.231948
6	1.609264	4.280123	-0.393770
1	0.593522	2.576330	0.443630
6	3.685208	3.814745	-1.539088
1	4.316793	1.759687	-1.560454
6	2.717047	4.729231	-1.118696
1	0.848362	4.983874	-0.067386
1	4.549635	4.155704	-2.102622
1	2.822283	5.783933	-1.357454
6	-2.514515	1.816098	-0.807883
6	-1.836719	2.091486	-2.008044
6	-3.352478	2.803782	-0.266554
6	-2.005481	3.314055	-2.660032
1	-1.163929	1.346671	-2.426384
6	-3.509030	4.034672	-0.911082

1	-3.884019	2.617325	0.661653
6	-2.840685	4.291116	-2.110341
1	-1.476019	3.507864	-3.589039
1	-4.156966	4.790431	-0.475185
1	-2.964362	5.247671	-2.610485
6	-2.824963	0.411354	1.720732
6	-4.163100	0.252325	2.116353
6	-1.873428	0.776641	2.688890
6	-4.539115	0.457286	3.446885
1	-4.914752	-0.035372	1.387440
6	-2.251589	0.991788	4.015625
1	-0.831090	0.881708	2.397390
6	-3.586127	0.829804	4.398064
1	-5.578161	0.327907	3.737669
1	-1.503411	1.276210	4.750692
1	-3.880743	0.988503	5.431734
6	-3.589693	-0.871995	-0.760331
6	-3.605168	-2.243761	-0.445792
6	-4.560746	-0.374007	-1.642609
6	-4.576063	-3.089157	-0.984623
1	-2.848272	-2.650892	0.220373
6	-5.525407	-1.225142	-2.192864
1	-4.570021	0.679522	-1.903352
6	-5.538243	-2.581656	-1.864151
1	-4.576065	-4.144356	-0.724719
1	-6.269089	-0.822212	-2.875261
1	-6.289431	-3.240345	-2.290991

Product Conctrans

ΔE_{DMF} -4811.95376663
ΔE_{DMF}(ZPE) -4811.363848
ΔG_{DMF} -4811.443444

6	-0.008168	2.147367	0.272439
1	-0.487102	2.568565	-0.617064
1	-0.605093	2.394669	1.154471
1	0.986633	2.582141	0.379804
46	0.012175	0.080657	0.056546
15	2.388410	0.223713	0.043211
15	-2.382698	0.119786	0.012076
35	-0.051609	-2.541424	-0.123597
6	3.344844	-1.250497	-0.520669
6	3.516101	-2.339266	0.351639
6	3.850918	-1.341061	-1.826310
6	4.196161	-3.482684	-0.068328
1	3.120043	-2.296649	1.361361
6	4.523697	-2.491965	-2.247105
1	3.730908	-0.514307	-2.518804
6	4.700819	-3.563267	-1.369864
1	4.328839	-4.311613	0.621371
1	4.914042	-2.543612	-3.259675
1	5.229399	-4.454667	-1.695715
6	2.990586	1.577204	-1.061246
6	4.111953	2.367269	-0.768627
6	2.291446	1.805613	-2.259082
6	4.528423	3.360403	-1.659568
1	4.661583	2.220026	0.154884
6	2.716112	2.790233	-3.153142
1	1.404428	1.219330	-2.484990
6	3.835639	3.571468	-2.853511
1	5.395066	3.968728	-1.416402
1	2.167232	2.951670	-4.076678
1	4.162102	4.343717	-3.544202
6	3.078433	0.568696	1.717287
6	4.445895	0.408442	2.006386
6	2.216273	0.999664	2.738809
6	4.937570	0.691224	3.281748
1	5.128733	0.050101	1.242055
6	2.711036	1.281083	4.014878
1	1.155123	1.106258	2.536538
6	4.071941	1.130542	4.287555
1	5.996149	0.563613	3.489445
1	2.030386	1.612320	4.794097
1	4.456558	1.346763	5.280220
6	-3.021237	-0.861685	-1.413100
6	-2.335270	-0.761882	-2.636123
6	-4.147647	-1.692556	-1.332229
6	-2.780096	-1.461196	-3.758875
1	-1.440452	-0.148557	-2.705835
6	-4.582929	-2.403101	-2.454619
1	-4.685476	-1.800481	-0.396453
6	-3.905130	-2.285946	-3.669697
1	-2.241146	-1.370549	-4.697849
1	-5.453016	-3.048800	-2.374809
1	-4.246554	-2.838532	-4.540414
6	-3.176880	-0.546882	1.535074
6	-4.552444	-0.379451	1.779634
6	-2.394207	-1.214015	2.490433
6	-5.130630	-0.883373	2.945563
1	-5.173614	0.154348	1.066747
6	-2.975264	-1.713529	3.659146
1	-1.331990	-1.347617	2.315276
6	-4.342967	-1.551755	3.887477
1	-6.194482	-0.748745	3.119238
1	-2.356076	-2.226441	4.389837
1	-4.793882	-1.939325	4.796690
6	-3.202484	1.766773	-0.180206
6	-3.627187	2.238900	-1.431985
6	-3.333072	2.608580	0.939205
6	-4.177663	3.517423	-1.559674
1	-3.540386	1.609929	-2.311861
6	-3.884662	3.884161	0.809078
1	-3.015076	2.266884	1.920004
6	-4.308186	4.342999	-0.441579
1	-4.508654	3.862169	-2.535346
1	-3.984812	4.517144	1.686350
1	-4.739150	5.335090	-0.541693

Adduct $S_N2$trans

ΔE_{DMF} -4811.91944377
ΔE_{DMF}(ZPE) -4811.330650
ΔG_{DMF} -4811.418619

6	1.676734	3.434144	0.332867
1	0.601099	3.393977	0.181669
1	2.205696	2.789957	-0.364072
1	1.946841	3.220611	1.363852
35	2.246115	5.293394	-0.040473
15	1.957464	-1.238234	-0.007170
46	-0.309546	-0.744332	0.002783
15	-2.553703	-0.160321	0.004869
6	-2.847771	1.666148	0.068953
6	-3.696996	2.282323	0.999357
6	-2.146019	2.473150	-0.845745
6	-3.842448	3.674176	1.014700
1	-4.247953	1.680985	1.715552
6	-2.304591	3.859384	-0.840063
1	-1.470927	2.011958	-1.562951
6	-3.150977	4.464700	0.095982
1	-4.501842	4.135921	1.744569
1	-1.764454	4.466714	-1.561418
1	-3.267726	5.544709	0.107082
6	-3.531791	-0.825250	1.426503
6	-4.905342	-1.107254	1.353049
6	-2.855218	-1.060135	2.635856
6	-5.585714	-1.608381	2.466017
1	-5.446654	-0.941772	0.426343
6	-3.538084	-1.551338	3.750208
1	-1.786804	-0.864528	2.694256
6	-4.905159	-1.828550	3.666258
1	-6.647829	-1.826034	2.393479
1	-3.000841	-1.726730	4.678239
1	-5.436272	-2.219674	4.529587
6	-3.515894	-0.695434	-1.480785
6	-4.569641	0.053854	-2.028188
6	-3.168867	-1.917504	-2.082594
6	-5.262672	-0.411944	-3.149123
1	-4.849016	1.004949	-1.584643
6	-3.868983	-2.386736	-3.195406
1	-2.339745	-2.494918	-1.679549
6	-4.916516	-1.633010	-3.732500
1	-6.074046	0.180195	-3.563565
1	-3.589457	-3.333898	-3.648624
1	-5.455851	-1.992772	-4.604296
6	2.393344	-2.907188	-0.673396
6	1.537022	-3.977998	-0.360916
6	3.520298	-3.152863	-1.473030
6	1.810564	-5.265987	-0.823007
1	0.649279	-3.795339	0.240825
6	3.785856	-4.441560	-1.946227
1	4.192540	-2.340293	-1.731568
6	2.935157	-5.499906	-1.620200
1	1.140894	-6.083462	-0.570075
1	4.660135	-4.615679	-2.567585
1	3.143338	-6.500345	-1.989148
6	2.973224	-0.074684	-1.026834
6	4.255193	0.361139	-0.657596
6	2.410438	0.411228	-2.220540
6	4.958328	1.261667	-1.464181
1	4.707809	0.005141	0.262659
6	3.117610	1.300746	-3.031489
1	1.409032	0.096616	-2.505376
6	4.393459	1.731541	-2.652192
1	5.948434	1.592546	-1.162724
1	2.669577	1.665067	-3.951909
1	4.941224	2.430906	-3.277575
6	2.780982	-1.198555	1.648894
6	3.845050	-2.042890	2.002810
6	2.311956	-0.267533	2.592287
6	4.429744	-1.953091	3.269550
1	4.219816	-2.773628	1.292285
6	2.903823	-0.171332	3.852995
1	1.473114	0.375546	2.335781
6	3.963540	-1.016573	4.194911
1	5.250450	-2.615766	3.530345
1	2.531673	0.555707	4.569702
1	4.419291	-0.948881	5.178805

TS $S_N2$trans

ΔE_{DMF} -4811.90667065
ΔE_{DMF}(ZPE) -4811.318903
ΔG_{DMF} -4811.403823

6	-0.013359	2.320736	0.058643
1	-0.769626	2.231605	-0.703642
1	1.025176	2.282763	-0.220682
1	-0.292996	2.207562	1.093848
35	-0.080247	4.682375	0.105818
15	2.344806	-0.434514	0.003657
46	0.008849	-0.246419	0.031667
15	-2.330013	-0.471683	0.007813
6	-3.279874	0.864056	-0.841969
6	-4.380212	1.513636	-0.264109
6	-2.838339	1.276214	-2.113352
6	-5.028303	2.549482	-0.944832
1	-4.736178	1.214999	0.716485
6	-3.492516	2.302954	-2.794866
1	-1.977105	0.792815	-2.569755
6	-4.588865	2.944760	-2.209344
1	-5.878017	3.044663	-0.483092
1	-3.141609	2.606680	-3.777139
1	-5.093708	3.749838	-2.735633
6	-3.105617	-0.617439	1.676483
6	-4.323165	-1.285507	1.888737
6	-2.446939	-0.039779	2.774303
6	-4.871260	-1.365565	3.170738
1	-4.842770	-1.749070	1.055140
6	-2.999601	-0.114959	4.054828
1	-1.492939	0.458847	2.623856
6	-4.212251	-0.778740	4.254844
1	-5.812459	-1.886923	3.321532
1	-2.478836	0.336936	4.894491
1	-4.639616	-0.844110	5.251482
6	-2.862250	-2.018345	-0.851500
6	-3.954502	-2.076217	-1.730196
6	-2.127166	-3.190783	-0.601466
6	-4.301948	-3.282125	-2.347217

1	-4.534496	-1.182722	-1.938535
6	-2.482853	-4.395280	-1.208930
1	-1.271906	-3.155824	0.069231
6	-3.569931	-4.442293	-2.087307
1	-5.148496	-3.311887	-3.027665
1	-1.907076	-5.293539	-1.003804
1	-3.842170	-5.377827	-2.567749
6	3.230056	0.763258	-1.087713
6	2.617894	1.109756	-2.305962
6	4.458788	1.353005	-0.753778
6	3.228546	2.013485	-3.176686
1	1.655790	0.673689	-2.565790
6	5.063540	2.266276	-1.622641
1	4.946414	1.104198	0.183400
6	4.452503	2.596274	-2.834203
1	2.743969	2.270081	-4.114560
1	6.013060	2.718271	-1.349745
1	4.923927	3.307652	-3.506338
6	3.188767	-0.292644	1.639141
6	4.381942	-0.970619	1.938408
6	2.611653	0.532654	2.618864
6	4.985946	-0.819554	3.188987
1	4.839146	-1.620712	1.198303
6	3.221019	0.688865	3.865463
1	1.678669	1.046872	2.405056
6	4.408778	0.011415	4.152831
1	5.907486	-1.351520	3.408543
1	2.764134	1.332138	4.612327
1	4.879828	0.126103	5.125022
6	2.873403	-2.093280	-0.613930
6	3.861207	-2.269661	-1.594054
6	2.238618	-3.227179	-0.075267
6	4.206467	-3.554204	-2.026682
1	4.363418	-1.408183	-2.022554
6	2.593067	-4.507684	-0.499949
1	1.464335	-3.104890	0.678690
6	3.576428	-4.673796	-1.480681
1	4.972112	-3.675693	-2.787970
1	2.097188	-5.374240	-0.071424
1	3.847028	-5.670517	-1.817507

Product $S_N2$trans

ΔE_{DMF} -4811.94083499
ΔE_{DMF}(ZPE) -4811.351581
ΔG_{DMF} -4811.438337

6	-0.041823	0.915435	1.555841
1	0.914950	1.415669	1.700182
1	-0.324650	0.360458	2.452725
1	-0.814663	1.638838	1.288890
35	-0.713773	6.031876	0.044883
15	-2.291470	-0.745224	0.031345
46	0.078987	-0.497054	0.080769
15	2.438758	-0.392785	0.037642
6	3.260653	-0.336301	1.676245
6	4.383059	0.464355	1.934963
6	2.722525	-1.121626	2.711637
6	4.961723	0.472057	3.207367
1	4.807418	1.082630	1.150698
6	3.309073	-1.117791	3.977114
1	1.841455	-1.731650	2.527982
6	4.428899	-0.318448	4.227255
1	5.828903	1.097796	3.397623
1	2.886471	-1.730185	4.768420
1	4.880077	-0.309084	5.215243
6	3.152094	0.967721	-0.966108
6	4.408218	0.838626	-1.583580
6	2.429829	2.162400	-1.119954
6	4.933141	1.891842	-2.334157
1	4.973776	-0.083297	-1.484896
6	2.960050	3.213857	-1.870656
1	1.451804	2.269780	-0.660903
6	4.210976	3.079949	-2.477613
1	5.904504	1.782375	-2.807740
1	2.391514	4.132172	-1.985133
1	4.620434	3.896787	-3.064940
6	3.012981	-1.935414	-0.777304
6	3.978536	-2.787062	-0.220603
6	2.420645	-2.276183	-2.007349
6	4.348276	-3.958045	-0.888638
1	4.443735	-2.540525	0.728397
6	2.796204	-3.443652	-2.671870
1	1.668346	-1.625583	-2.447476
6	3.760440	-4.287511	-2.111846
1	5.100044	-4.609147	-0.451849
1	2.335205	-3.694680	-3.622754
1	4.051408	-5.198043	-2.627526
6	-2.656378	-2.454290	-0.541464
6	-2.002238	-2.902207	-1.703889
6	-3.525979	-3.323586	0.133353
6	-2.219582	-4.193584	-2.183895
1	-1.327861	-2.237480	-2.238478
6	-3.737187	-4.618672	-0.349166
1	-4.039270	-2.996275	1.031543
6	-3.086629	-5.055386	-1.504880
1	-1.711445	-4.526237	-3.084394
1	-4.415478	-5.282601	0.179102
1	-3.254020	-6.062145	-1.876498
6	-3.185234	-0.539514	1.619605
6	-4.343177	0.243365	1.736104
6	-2.667340	-1.174786	2.763198
6	-4.976103	0.382106	2.974726
1	-4.754910	0.743816	0.865899
6	-3.307898	-1.041159	3.994964
1	-1.762776	-1.773828	2.691400
6	-4.462495	-0.259557	4.102944
1	-5.871150	0.992403	3.053188
1	-2.901081	-1.539770	4.869957
1	-4.956372	-0.149524	5.064042
6	-3.122931	0.343721	-1.191596
6	-4.329845	-0.031097	-1.807025
6	-2.537610	1.576960	-1.521936
6	-4.940595	0.818800	-2.730430
1	-4.789692	-0.986348	-1.571443
6	-3.153779	2.425538	-2.444391
1	-1.597557	1.871249	-1.065375
6	-4.354718	2.047470	-3.049001
1	-5.872768	0.520058	-3.201189
1	-2.690580	3.375774	-2.693590
1	-4.831117	2.705560	-3.769978

2.2 Mono-phosphine Palladium catalyst

2.2.1 Species Optimized in gas phase

2.2.1.1 PF_3

$PdPF_3$

ΔE_{gas} -768.931563744
ΔE_{gas}(ZPE) -768.921957
ΔG_{gas} -768.952512

46	0.000000	0.000000	1.272141
15	0.000000	0.000000	-0.872953
9	0.000000	1.385994	-1.682379
9	-1.200306	-0.692997	-1.682379
9	1.200306	-0.692997	-1.682379

PF_3

ΔE_{gas} -640.983166692
ΔE_{gas}(ZPE) -640.975021
ΔG_{gas} -641.001256

15	0.000000	0.000000	0.514183
9	0.000000	1.397221	-0.285657
9	-1.210029	-0.698611	-0.285657
9	1.210029	-0.698611	-0.285657

Adduct Conc2

ΔE_{gas} -3380.28531220
ΔE_{gas}(ZPE) -3380.237507
ΔG_{gas} -3380.279817

6	3.162385	1.484822	-0.000335
1	2.769567	1.963878	0.892471
1	4.248141	1.420882	0.014740
1	2.793815	1.950747	-0.910279
15	-2.192283	0.068017	0.001366
46	-0.050635	-0.122351	-0.007017
35	2.501478	-0.386709	0.004584
9	-2.880123	1.478390	-0.350352
9	-3.034136	-0.215036	1.341551
9	-3.099534	-0.830215	-0.974872

TS Conc2

ΔE_{gas} -3380.25300975
ΔE_{gas}(ZPE) -3380.207339
ΔG_{gas} -3380.246969

15	-2.006201	-0.149280	0.000032
46	0.112717	0.510783	-0.000009
35	2.316790	-0.731763	-0.000036
6	2.035458	1.561461	-0.000017
1	2.601237	1.725584	0.909636
1	2.601187	1.725607	-0.909697
1	1.091710	2.190357	0.000026
9	-2.549017	-1.052639	1.203605
9	-2.549017	-1.052821	-1.203402
9	-3.200462	0.921522	-0.000050

Product Conc2

ΔE_{gas} -3380.26862811
ΔE_{gas}(ZPE) -3380.222631
ΔG_{gas} -3380.263570

15	1.790273	-0.077828	-0.000003
46	-0.383821	0.859756	0.000068
35	-1.600410	-1.252052	0.000000
6	-2.206036	1.726005	-0.000161
1	-2.772180	1.501430	-0.903468
1	-2.775634	1.497845	0.900028
1	-1.813469	2.759978	0.002768
9	2.205153	-1.028695	-1.204624
9	3.079596	0.870593	-0.000549
9	2.205642	-1.027992	1.205011

Adduct Conc1

ΔE_{gas} -3380.28531214
ΔE_{gas}(ZPE) -3380.237507
ΔG_{gas} -3380.279815

15	-2.192301	0.068026	0.001396
46	-0.050624	-0.122221	-0.006911
35	2.501406	-0.386755	0.004543
6	3.162710	1.484645	-0.000361
1	4.248443	1.420475	0.015218
1	2.794651	1.950498	-0.910549
1	2.769577	1.963919	0.892186
9	-3.099254	-0.830837	-0.974543
9	-3.034326	-0.214456	1.341593
9	-2.880299	1.478119	-0.351129

TS Conc1

ΔE_{gas} -3380.25552694
ΔE_{gas}(ZPE) -3380.209487
ΔG_{gas} -3380.250968

6	1.454387	1.870074	-0.000514
1	1.188763	2.076161	1.030695
1	2.430855	2.233992	-0.287875
1	0.690766	2.085510	-0.743796
15	-2.056135	-0.026348	0.003821
46	0.125032	-0.202579	-0.014132
35	2.546869	-0.266248	0.009070
9	-2.730863	1.376588	-0.386231
9	-2.876290	-0.267142	1.358642
9	-2.958023	-0.952062	-0.941371

Product Conc1

ΔE_{gas} -3380.28942809
ΔE_{gas}(ZPE) -3380.242098
ΔG_{gas} -3380.282241

46	-0.234341	-0.066007	0.000044
15	1.987026	-0.158840	-0.000005
6	-0.178196	1.996464	-0.000015
1	0.344242	2.293282	-0.910478
1	-1.217864	2.312584	0.000162
1	0.344578	2.293366	0.910228
35	-2.623836	-0.226546	-0.000022
9	2.658621	-1.598885	-0.000484
9	2.804438	0.491834	1.199756
9	2.804360	0.492606	-1.199387

Adduct S_N21

ΔE_{gas} -3380.26425353
ΔE_{gas}(ZPE) -3380.217179
ΔG_{gas} -3380.260568

6	2.056688	0.948529	-0.000797
1	1.492549	0.789965	-0.936412
1	1.493424	0.792008	0.935636
1	2.447322	1.963538	-0.001982
35	3.558390	-0.308465	-0.000062
15	-2.485432	-0.127208	-0.000114
46	-0.358402	0.225077	0.000495
9	-3.172286	-0.925237	1.208412
9	-3.166717	-0.953565	-1.192594
9	-3.499786	1.113712	-0.017081

TS S_N21

ΔE_{gas} -3380.19666909
ΔE_{gas}(ZPE) -3380.152896
ΔG_{gas} -3380.196093

6	0.733299	1.313878	0.014532
1	0.562668	1.917145	-0.878639
1	1.656600	0.648857	-0.016109
1	0.603907	1.880271	0.938578
35	3.610124	0.026523	-0.007528
15	-2.402915	0.061348	-0.004640
46	-0.278279	-0.468662	0.012049
9	-3.132818	0.353267	1.374947
9	-3.474319	-0.924271	-0.643950
9	-2.807612	1.391047	-0.770129

Product S_N21

ΔE_{gas} -3380.28942809
ΔE_{gas}(ZPE) -3380.242098
ΔG_{gas} -3380.282241

46	-0.234341	-0.066007	0.000044
15	1.987026	-0.158840	-0.000005
6	-0.178196	1.996464	-0.000015
1	0.344242	2.293282	-0.910478
1	-1.217864	2.312584	0.000162
1	0.344578	2.293366	0.910228
35	-2.623836	-0.226546	-0.000022
9	2.658621	-1.598885	-0.000484
9	2.804438	0.491834	1.199756
9	2.804360	0.492606	-1.199387

Adduct S_N22

ΔE_{gas} -3380.26426489
ΔE_{gas}(ZPE) -3380.217202
ΔG_{gas} -3380.260775

6	-2.050469	-0.936611	0.008231
1	-2.423053	-1.958315	0.014918
1	-1.490622	-0.774165	-0.929542
1	-1.489356	-0.761471	0.942439
35	-3.573842	0.293980	0.000454
15	2.492854	0.119136	0.000911
46	0.360831	-0.201976	-0.004397
9	3.335970	-0.111646	1.344662
9	3.097283	1.557522	-0.364223
9	3.433333	-0.742748	-0.969830

TS S_N22

ΔE_{gas} -3380.18151873
ΔE_{gas}(ZPE) -3380.138721
ΔG_{gas} -3380.181773

6	1.414152	1.943897	-0.000351
1	1.524986	2.541130	0.908499
1	1.525062	2.539452	-0.910299
1	1.931172	0.949982	0.000536
35	3.220340	-0.769012	0.000046
46	-0.346838	0.902100	0.000058
15	-2.220525	-0.480511	-0.000029
9	-2.034384	-2.057015	-0.048318
9	-3.231491	-0.397839	1.228958
9	-3.280304	-0.330418	-1.180690

Product S_N22

ΔE_{gas} -3380.26862811
ΔE_{gas}(ZPE) -3380.222631
ΔG_{gas} -3380.263570

15	1.790273	-0.077828	-0.000003
46	-0.383821	0.859756	0.000068
35	-1.600410	-1.252052	0.000000
6	-2.206036	1.726005	-0.000161
1	-2.772180	1.501430	-0.903468
1	-2.775634	1.497845	0.900028
1	-1.813469	2.759978	0.002768
9	2.205153	-1.028695	-1.204624
9	3.079596	0.870593	-0.000549
9	2.205642	-1.027992	1.205011

2.2.1.2 PH_3

$PdPH_3$

ΔE_{gas} -471.087272642
ΔE_{gas}(ZPE) -471.060418
ΔG_{gas} -471.087299

46	-0.651673	0.000000	0.000004
15	1.544727	0.000007	0.000036
1	2.268542	1.121919	-0.479427
1	2.269184	-0.146010	1.210926
1	2.268311	-0.976036	-0.732232

PH_3

ΔE_{gas} -343.144519272
ΔE_{gas}(ZPE) -343.120491
ΔG_{gas} -343.141536

15	-0.000017	0.000010	-0.128110
1	-0.085559	1.195365	0.640618
1	-0.992450	-0.671920	0.640604
1	1.078267	-0.523593	0.640421

Adduct Conc2

ΔE_{gas} -3082.43739685
ΔE_{gas}(ZPE) -3082.372471
ΔG_{gas} -3082.409016

46	0.710713	-0.042667	0.000438
35	-1.803779	-0.419139	-0.000249
15	2.916924	0.174298	-0.000562
1	3.516566	1.460586	0.003699
1	3.705424	-0.359668	1.051642
1	3.704033	-0.352126	-1.057596
6	-2.648406	1.379272	-0.000079
1	-3.275010	1.433338	-0.887525
1	-3.232459	1.453619	0.914472
1	-1.842471	2.106714	-0.027247

TS Conc2

ΔE_{gas} -3082.41119823
ΔE_{gas}(ZPE) -3082.348351
ΔG_{gas} -3082.384238

15	-2.708320	-0.447460	-0.000013
46	-0.557416	0.292199	0.000006
35	1.847584	-0.570041	0.000000
1	-3.811532	0.443982	-0.000085
1	-3.172774	-1.267732	-1.057426
1	-3.172729	-1.267524	1.057580
6	1.304618	1.591833	-0.000014
1	1.831474	1.861971	0.908026
1	1.831245	1.861967	-0.908188
1	0.267112	2.038497	0.000123

Product Conc2

ΔE_{gas} -3082.43655555
ΔE_{gas}(ZPE) -3082.373260
ΔG_{gas} -3082.409515

15	2.257810	-0.808789	0.000015
46	0.347621	0.724818	0.000022
35	-1.337696	-1.038939	-0.000044
1	3.627526	-0.443222	0.000037
1	2.313264	-1.734518	1.064917
1	2.313287	-1.734475	-1.064924
6	-1.186646	2.033850	0.000029
1	-1.798166	1.953433	-0.899430
1	-1.798181	1.953400	0.899476
1	-0.576196	2.955350	0.000051

Adduct Conc1

ΔE_{gas} -3082.43735390
ΔE_{gas}(ZPE) -3082.372513
ΔG_{gas} -3082.407326

15	2.909396	0.211122	0.001649
46	0.711883	-0.076810	-0.001371
35	-1.812854	-0.405049	0.000914
1	3.460257	1.518211	0.030906
1	3.718517	-0.313389	1.042661
1	3.714660	-0.264969	-1.065565
6	-2.605965	1.415227	-0.000177
1	-3.253815	1.477510	-0.872217
1	-3.163819	1.519253	0.928010
1	-1.777663	2.115170	-0.056396

TS Conc1

ΔE_{gas} -3082.41209657
ΔE_{gas} (ZPE) -3082.348932
ΔG_{gas} -3082.387780

6	0.989032	1.834187	0.001640
1	0.592923	2.061061	0.986541
1	1.997960	2.194713	-0.147953
1	0.334035	2.069165	-0.833547
15	-2.773593	-0.009785	0.009682
46	-0.518782	-0.138735	-0.008440
35	1.917046	-0.310064	0.005037
1	-3.539930	-1.201373	0.053717
1	-3.486438	0.594767	-1.056385
1	-3.461510	0.657343	1.054477

Product Conc1

ΔE_{gas} -3082.45577974
ΔE_{gas}(ZPE) -3082.391238
ΔG_{gas} -3082.425554

6	-0.562259	1.904636	0.000003
1	-1.105110	2.180845	0.906468
1	-1.104498	2.180756	-0.906859
1	0.451016	2.299596	0.000323
35	2.050108	-0.153463	-0.000001
15	-2.650671	-0.372884	-0.000007
1	-3.262993	-1.068056	1.068189
1	-3.474262	0.775361	-0.000685
1	-3.262968	-1.069297	-1.067408
46	-0.366551	-0.125273	0.000002

Adduct S_N21

ΔE_{gas} -3082.42168225
ΔE_{gas}(ZPE) -3082.357447
ΔG_{gas} -3082.396086

6	-1.270138	0.876865	0.000677
1	-0.723136	0.657376	-0.933729
1	-0.723650	0.657215	0.935247
1	-1.577860	1.919220	0.000595
35	-2.885812	-0.241661	0.000043
46	1.100250	0.131072	-0.000365
15	3.273783	-0.312801	0.000454
1	4.100131	0.139395	1.059186
1	3.729024	-1.654715	-0.000376
1	4.101460	0.141148	-1.056492

TS S_N21

ΔE_{gas} -3082.36888970
ΔE_{gas}(ZPE) -3082.307121
ΔG_{gas} -3082.344341

6	0.056154	1.235880	-0.000513
1	-0.081411	1.828665	0.906849
1	-0.081465	1.828317	-0.908100
1	0.992549	0.599537	-0.000435
35	3.023804	0.029778	0.000138
15	-3.135483	0.407338	0.000324
1	-4.002991	0.119670	1.076756
1	-3.233943	1.814061	-0.000290
1	-4.004518	0.118644	-1.074602
46	-1.059262	-0.453836	-0.000147

Product S_N21

ΔE_{gas} -3082.45577974
ΔE_{gas}(ZPE) -3082.391238
ΔG_{gas} -3082.425554

6	-0.562259	1.904636	0.000003
1	-1.105110	2.180845	0.906468
1	-1.104498	2.180756	-0.906859
1	0.451016	2.299596	0.000323
35	2.050108	-0.153463	-0.000001
15	-2.650671	-0.372884	-0.000007
1	-3.262993	-1.068056	1.068189
1	-3.474262	0.775361	-0.000685
1	-3.262968	-1.069297	-1.067408
46	-0.366551	-0.125273	0.000002

Adduct S_N22

ΔE_{gas} -3082.42168225
ΔE_{gas}(ZPE) -3082.357447
ΔG_{gas} -3082.396086

6	-1.270138	0.876865	0.000677
1	-0.723136	0.657376	-0.933729
1	-0.723650	0.657215	0.935247
1	-1.577860	1.919220	0.000595
35	-2.885812	-0.241661	0.000043
46	1.100250	0.131072	-0.000365
15	3.273783	-0.312801	0.000454
1	4.100131	0.139395	1.059186
1	3.729024	-1.654715	-0.000376
1	4.101460	0.141148	-1.056492

TS S_N22

ΔE_{gas} -3082.35186927
ΔE_{gas}(ZPE) -3082.291725
ΔG_{gas} -3082.330840

6	0.453653	1.808274	-0.000027
1	0.474787	2.419654	0.906992
1	0.474783	2.419571	-0.907103
1	1.149269	0.930338	0.000001
35	2.809209	-0.492100	0.000001
46	-1.110116	0.516519	0.000009
15	-2.813394	-1.201595	-0.000017
1	-3.738172	-1.293960	1.065187
1	-3.744930	-1.287764	-1.059848
1	-2.393708	-2.549944	-0.005268

Product S_N22

ΔE_{gas} -3082.43655555
ΔE_{gas}(ZPE) -3082.373260
ΔG_{gas} -3082.409515

15	2.257810	-0.808789	0.000015
46	0.347621	0.724818	0.000022
35	-1.337696	-1.038939	-0.000044
1	3.627526	-0.443222	0.000037
1	2.313264	-1.734518	1.064917
1	2.313287	-1.734475	-1.064924
6	-1.186646	2.033850	0.000029
1	-1.798166	1.953433	-0.899430
1	-1.798181	1.953400	0.899476
1	-0.576196	2.955350	0.000051

2.2.1.3 $P(CH_3)_3$

$PdP(CH_3)_3$

ΔE_{gas} -589.064149833
ΔE_{gas} (ZPE) -588.949835
ΔG_{gas} -588.983395

46	-1.327963	0.000007	0.000166
15	0.880112	0.000152	-0.000261
6	1.720182	-1.401490	-0.878180
1	1.407194	-1.413766	-1.926296
1	2.812722	-1.311136	-0.827874
1	1.415446	-2.349192	-0.424789
6	1.721544	-0.060213	1.651787
1	1.411970	-0.964138	2.184443
1	2.814147	-0.057736	1.547743
1	1.414180	0.803833	2.248105
6	1.720442	1.461393	-0.774135
1	1.410850	2.374002	-0.256616
1	2.813051	1.370786	-0.725064
1	1.412046	1.546605	-1.820204

$P(CH_3)_3$

ΔE_{gas} -461.113076767
ΔE_{gas}(ZPE) -461.000579
ΔG_{gas} -461.029939

15	-0.000103	-0.000185	-0.602565
6	-1.556158	-0.532300	0.279703
1	-1.814369	-1.554107	-0.018173
1	-1.456909	-0.497814	1.372068
1	-2.385480	0.117790	-0.018783
6	0.316970	1.613594	0.279486
1	-0.438638	2.348147	-0.018650
1	0.296204	1.509700	1.371769
1	1.294931	2.006695	-0.018099
6	1.239399	-1.081062	0.279628
1	2.253019	-0.795068	-0.020740
1	1.161656	-1.008940	1.371869
1	1.089872	-2.125027	-0.015697

Adduct Conc2

ΔE_{gas} -3200.41404601
ΔE_{gas}(ZPE) -3200.261666
ΔG_{gas} -3200.305415

15	2.234053	0.062234	0.000066
46	-0.001551	-0.078839	0.000037
35	-2.512394	-0.403543	-0.000017
6	-3.305021	1.415670	0.000032
1	-2.957946	1.914905	-0.900981
1	-4.385528	1.285599	0.002746
1	-2.953910	1.916627	0.898558
6	3.132931	-0.711297	-1.427945
1	2.802851	-0.244925	-2.360481
1	4.219507	-0.596132	-1.330642
1	2.887108	-1.775770	-1.478168
6	2.976807	1.763806	-0.002975
1	4.073207	1.726242	-0.003197
1	2.636016	2.307537	-0.888649
1	2.636454	2.310726	0.880903
6	3.133053	-0.706333	1.430667
1	4.219629	-0.591637	1.332799
1	2.803191	-0.236566	2.361583
1	2.887124	-1.770585	1.484739

TS Conc2

ΔE_{gas} -3200.38895786
ΔE_{gas}(ZPE) -3200.238633
ΔG_{gas} -3200.280103

15	2.095728	-0.127993	-0.000258
46	-0.122508	0.425660	0.000994
35	-2.469556	-0.647590	-0.000288
6	-2.126961	1.527328	-0.002541
1	-2.669557	1.764937	-0.910848
1	-2.672969	1.767061	0.903176
1	-1.121881	2.049666	-0.001081
6	2.654166	-1.275324	-1.345102
1	2.457940	-0.818472	-2.319271
1	3.723929	-1.501371	-1.262404
1	2.083241	-2.206332	-1.287940
6	3.340535	1.239018	-0.162249
1	4.366774	0.852674	-0.155025
1	3.167850	1.780604	-1.096697
1	3.216759	1.944153	0.664725
6	2.725348	-1.004511	1.506533
1	3.790406	-1.247690	1.413844
1	2.576460	-0.372252	2.386430
1	2.156417	-1.926852	1.653501

Product Conc2

ΔE_{gas} -3200.41808414
ΔE_{gas}(ZPE) -3200.267352
ΔG_{gas} -3200.309254

15	-1.817793	0.050425	0.000262
46	0.435565	-0.888447	-0.000589
35	1.585930	1.268984	0.000519
6	2.272187	-1.742209	-0.001360
1	2.844233	-1.506319	-0.900276
1	2.845891	-1.505668	0.896307
1	1.935661	-2.795899	-0.000625
6	-2.143101	1.158738	-1.439935
1	-2.113818	0.577136	-2.365956
1	-3.116986	1.653075	-1.354915
1	-1.351035	1.910967	-1.485299
6	-3.306123	-1.055594	-0.000635
1	-4.235514	-0.475347	-0.000040
1	-3.291363	-1.696505	-0.887416
1	-3.291189	-1.698006	0.885064
6	-2.143086	1.156145	1.442465
1	-3.117006	1.650569	1.358354
1	-2.113720	0.572895	2.367444
1	-1.351077	1.908354	1.489160

Adduct Conc1

ΔE_{gas} -3200.41405596
ΔE_{gas}(ZPE) -3200.261674
ΔG_{gas} -3200.305415

15	-2.230374	0.064487	0.000950
46	0.003858	-0.100543	0.000222
35	2.517804	-0.395486	0.001598
6	3.262039	1.444066	-0.003473
1	4.345628	1.342772	-0.002366
1	2.900016	1.931595	-0.904958
1	2.898554	1.936947	0.894495
6	-3.157646	-0.983305	-1.218865
1	-4.241699	-0.842890	-1.129012
1	-2.843644	-0.721436	-2.233102
1	-2.915442	-2.036448	-1.052075
6	-3.121280	-0.361606	1.573066
1	-4.207029	-0.249923	1.464428
1	-2.891648	-1.393383	1.853234
1	-2.770466	0.292017	2.376534
6	-2.956673	1.735095	-0.358983
1	-4.052970	1.707854	-0.337740
1	-2.600991	2.454233	0.384060
1	-2.623978	2.072866	-1.344342

TS Conc1

ΔE_{gas} -3200.38984783
ΔE_{gas}(ZPE) -3200.239217
ΔG_{gas} -3200.281220

6	-1.804953	1.824361	0.000031
1	-0.749147	2.092602	-0.001006
1	-2.318823	2.095632	-0.913273
1	-2.317050	2.095400	0.914401
15	2.127377	-0.013358	0.000030
46	-0.149779	-0.112828	-0.000055
35	-2.581779	-0.343242	0.000028
6	2.932705	1.657676	-0.001657
1	2.615954	2.215136	-0.888108
1	2.615982	2.216975	0.883647
1	4.026310	1.579230	-0.001597
6	2.984860	-0.819430	1.432967
1	4.075231	-0.748618	1.341113
1	2.669826	-0.339424	2.363811
1	2.696098	-1.873063	1.483051
6	2.984968	-0.822330	-1.431216
1	2.669993	-0.344219	-2.363054
1	4.075335	-0.751324	-1.339432
1	2.696223	-1.876066	-1.479180

Product Conc1

ΔE_{gas} -3200.44119873
ΔE_{gas}(ZPE) -3200.289207
ΔG_{gas} -3200.330852

6	-0.144992	2.019241	0.000317
1	0.214305	2.324420	-0.985411
1	0.521718	2.355002	0.797924
1	-1.165613	2.358401	0.171741
35	-2.687063	-0.249120	0.001569
15	2.022392	-0.165209	-0.000007
46	-0.263089	-0.012369	-0.002747
6	2.596785	-1.897267	-0.286698
1	2.234866	-2.249556	-1.256581
1	3.690571	-1.953961	-0.269649
1	2.193637	-2.554236	0.489188
6	2.873699	0.300218	1.569818
1	2.481361	-0.307354	2.389750
1	3.956210	0.150732	1.494031
1	2.674092	1.350399	1.800194
6	2.946573	0.795633	-1.274563
1	4.024102	0.614927	-1.199278
1	2.601138	0.506737	-2.270916
1	2.754658	1.863845	-1.142707

Adduct $S_N2$1

ΔE_{gas} -3200.39946213
ΔE_{gas}(ZPE) -3200.247873
ΔG_{gas} -3200.289685

6	2.063584	-0.892918	-0.000456
1	2.424154	-1.918006	-0.005037
1	1.507775	-0.701420	0.935438
1	1.503160	-0.695075	-0.932642
35	3.626001	0.303055	-0.000519
15	-2.528677	0.132231	0.000109
46	-0.324007	-0.255554	0.002225
6	-3.516466	-0.663695	-1.351592
1	-4.581102	-0.414287	-1.268333
1	-3.142832	-0.326815	-2.322541
1	-3.396056	-1.749374	-1.300944
6	-3.479802	-0.395289	1.501427
1	-4.545811	-0.156597	1.403090
1	-3.364088	-1.472896	1.646950
1	-3.077675	0.110385	2.383696
6	-3.057770	1.901466	-0.158266
1	-2.668355	2.316737	-1.091840
1	-4.150608	1.993081	-0.149933
1	-2.641432	2.481975	0.669607

TS $S_N2$1

ΔE_{gas} -3200.35738529
ΔE_{gas}(ZPE) -3200.207820

ΔG_{gas} -3200.250397

6	0.717597	1.051640	0.000372
1	0.563050	1.641788	0.907194
1	0.563308	1.641839	-0.906457
1	1.692605	0.483950	0.000468
35	3.811319	0.120751	-0.000090
15	-2.456656	0.183123	-0.000080
46	-0.363426	-0.653113	0.000081
6	-2.868200	1.241813	1.449141
1	-3.899716	1.604523	1.381521
1	-2.745212	0.668969	2.371824
1	-2.187839	2.096470	1.483466
6	-2.867625	1.243002	-1.448585
1	-3.899177	1.605630	-1.381075
1	-2.187265	2.097696	-1.481915
1	-2.744256	0.670930	-2.371697
6	-3.785657	-1.096928	-0.000867
1	-3.694102	-1.729221	0.886287
1	-4.772911	-0.621336	-0.000742
1	-3.693893	-1.728331	-0.888632

Product S_N21

ΔE_{gas} -3200.44119871
ΔE_{gas}(ZPE) -3200.289209
ΔG_{gas} -3200.330860

6	0.144876	2.019280	0.000281
1	-0.523302	2.355198	0.796577
1	-0.212416	2.324305	-0.986216
1	1.165191	2.358375	0.173665
35	2.687121	-0.249128	0.001502
15	-2.022394	-0.165236	0.000020
46	0.263067	-0.012349	-0.002570
6	-2.874103	0.300025	1.569664
1	-3.956608	0.150700	1.493474
1	-2.482130	-0.307769	2.389603
1	-2.674442	1.350136	1.800308
6	-2.946231	0.795755	-1.274675
1	-4.023787	0.615077	-1.199672
1	-2.754308	1.863944	-1.142666
1	-2.600547	0.506920	-2.270954
6	-2.596732	-1.897251	-0.287023
1	-2.193993	-2.554325	0.488984
1	-3.690530	-1.953860	-0.270488
1	-2.234412	-2.249471	-1.256783

Adduct S_N22

ΔE_{gas} -3200.39946166
ΔE_{gas}(ZPE) -3200.247870
ΔG_{gas} -3200.289681

6	-2.063522	-0.892868	-0.001592
1	-1.508165	-0.702776	0.934874
1	-1.502662	-0.693650	-0.933225
1	-2.424064	-1.917973	-0.007781
35	-3.625940	0.303149	-0.000570
46	0.323998	-0.255759	0.002843
15	2.528592	0.132297	-0.000057
6	3.057392	1.902728	-0.145669
1	4.150258	1.994092	-0.139208
1	2.665821	2.325453	-1.074976
1	2.643117	2.476688	0.687789
6	3.514064	-0.653006	-1.359648
1	3.138801	-0.308504	-2.327283
1	4.578845	-0.404265	-1.276208
1	3.393731	-1.739042	-1.317333
6	3.482445	-0.406732	1.495442
1	4.548168	-0.166752	1.397223
1	3.081535	0.091752	2.382339
1	3.367479	-1.485507	1.632637

TS S_N22

ΔE_{gas} -3200.33364579
ΔE_{gas}(ZPE) -3200.185976
ΔG_{gas} -3200.230103

6	-1.429201	-1.923179	0.003416
1	-1.948200	-0.929043	-0.001906
1	-1.575307	-2.513505	0.913284
1	-1.576578	-2.524561	-0.898880
46	0.341387	-0.935716	-0.002013
15	2.321192	0.476162	-0.000625
6	3.973492	-0.340418	-0.168412
1	4.783845	0.396585	-0.154631
1	4.122400	-1.047223	0.653139
1	4.016539	-0.897488	-1.108897
6	2.364871	1.743456	-1.345117
1	3.256685	2.374674	-1.266304
1	2.361578	1.247889	-2.320134
1	1.471889	2.371481	-1.281531
6	2.537089	1.502883	1.521125
1	2.643384	0.852648	2.394158
1	3.420006	2.146734	1.444495
1	1.650045	2.125457	1.667882
35	-3.366442	0.754297	-0.000136

Product S_N22

ΔE_{gas} -3200.41808414
ΔE_{gas}(ZPE) -3200.267352
ΔG_{gas} -3200.309254

15	-1.817793	0.050425	0.000262
46	0.435565	-0.888447	-0.000589
35	1.585930	1.268984	0.000519
6	2.272187	-1.742209	-0.001360
1	2.844233	-1.506319	-0.900276
1	2.845891	-1.505668	0.896307
1	1.935661	-2.795899	-0.000625
6	-2.143101	1.158738	-1.439935
1	-2.113818	0.577136	-2.365956
1	-3.116986	1.653075	-1.354915
1	-1.351035	1.910967	-1.485299
6	-3.306123	-1.055594	-0.000635
1	-4.235514	-0.475347	-0.000040
1	-3.291363	-1.696505	-0.887416
1	-3.291189	-1.698006	0.885064
6	-2.143086	1.156145	1.442465
1	-3.117006	1.650569	1.358354
1	-2.113720	0.572895	2.367444
1	-1.351077	1.908354	1.489160

2.2.1.4 PPh_3

$PdPPh_3$

ΔE_{gas} -1164.23464631
ΔE_{gas} (ZPE) -1163.959170
ΔG_{gas} -1164.008497

15	0.000594	-0.001531	0.364628
6	-0.381411	1.638042	-0.412666
6	1.598919	-0.489388	-0.440208
6	-1.231924	-1.138358	-0.425752
6	-2.486625	-1.281670	0.191579
6	-3.462987	-2.110664	-0.361767
6	-3.193747	-2.824808	-1.533343
6	-1.947412	-2.698469	-2.149739
6	-0.973223	-1.857437	-1.603193
1	-2.687770	-0.744813	1.116054
1	-4.428680	-2.207833	0.127022
1	-3.949210	-3.479291	-1.959398
1	-1.729492	-3.253024	-3.058639
1	-0.010242	-1.765425	-2.095990
6	2.087763	0.109832	-1.611411
6	3.302987	-0.303525	-2.166346
6	4.040202	-1.324841	-1.564329
6	3.560654	-1.930948	-0.399038
6	2.355099	-1.509850	0.162361
1	1.522791	0.901448	-2.093758
1	3.670642	0.174891	-3.070254
1	4.984859	-1.643715	-1.996231
1	4.131091	-2.722775	0.079030
1	1.995950	-1.965586	1.082442
6	0.131313	2.793535	0.201776
6	-0.104610	4.056040	-0.343478
6	-0.873484	4.185240	-1.503825
6	-1.397817	3.045675	-2.116977
6	-1.151055	1.779205	-1.578531
1	0.710642	2.695027	1.117162
1	0.301782	4.938574	0.143279
1	-1.067064	5.168609	-1.923543
1	-2.000051	3.138304	-3.016878
1	-1.563496	0.902353	-2.068192
46	0.018989	-0.020422	2.566909

PPh_3

ΔE_{gas} -1036.28400510
ΔE_{gas}(ZPE) -1036.009737
ΔG_{gas} -1036.055374

15	-0.000399	-0.001583	-1.198073
6	0.377709	1.630299	-0.404015
6	1.283955	2.470370	-1.075196
6	-0.191730	2.080804	0.797592
6	1.627793	3.717317	-0.550180
1	1.719712	2.147509	-2.017995
6	0.144966	3.333089	1.318535
1	-0.899461	1.453241	1.330669
6	1.057302	4.152138	0.649247
1	2.331825	4.351579	-1.081588
1	-0.305709	3.666699	2.249315
1	1.316591	5.125626	1.055630
6	-1.602268	-0.487923	-0.402252
6	-1.707895	-1.202488	0.801879
6	-2.782813	-0.126036	-1.075340
6	-2.961008	-1.537956	1.321955
1	-0.810571	-1.497522	1.337276
6	-4.034716	-0.450499	-0.549908
1	-2.720725	0.410004	-2.019585
6	-4.126126	-1.160597	0.650421
1	-3.025065	-2.092372	2.254299
1	-4.936174	-0.159703	-1.082037
1	-5.098880	-1.422957	1.056643
6	1.223357	-1.143294	-0.402193
6	1.495588	-2.349848	-1.071690
6	1.901136	-0.873039	0.797072
6	2.404393	-3.270261	-0.546863
1	0.995222	-2.567866	-2.012429
6	2.820010	-1.789092	1.316568
1	1.710822	0.053742	1.329430
6	3.071195	-2.989966	0.649057
1	2.599316	-4.198768	-1.076193
1	3.337483	-1.563654	2.245069
1	3.786524	-3.699922	1.054462

Adduct Conc2

ΔE_{gas} -3775.58501311
ΔE_{gas}(ZPE) -3775.271469
ΔG_{gas} -3775.328714

6	-4.866622	1.350387	-0.157000
1	-5.947013	1.221982	-0.183578
1	-4.549316	1.945381	0.695594
1	-4.481358	1.749356	-1.091776
15	0.669642	-0.007195	0.004324
46	-1.574008	-0.142505	0.034022
35	-4.083175	-0.458141	0.070400
6	1.501856	-1.116126	-1.223974
6	0.855203	-1.330044	-2.452855
6	2.730768	-1.750946	-0.988303
6	1.432161	-2.142517	-3.428746
1	-0.111518	-0.864551	-2.629908
6	3.301496	-2.575144	-1.962106
1	3.241869	-1.610493	-0.040624
6	2.656772	-2.769597	-3.184515
1	0.919195	-2.296334	-4.374584
1	4.250769	-3.065483	-1.761680
1	3.101423	-3.412300	-3.939836
6	1.519316	-0.423980	1.596744
6	2.685605	0.217432	2.041597
6	0.956599	-1.434054	2.394718
6	3.277387	-0.147562	3.253886
1	3.130363	1.009427	1.446349
6	1.555049	-1.805391	3.598702
1	0.038114	-1.916511	2.069004
6	2.716361	-1.160862	4.032644
1	4.177126	0.362863	3.588050
1	1.107579	-2.589618	4.203793
1	3.176832	-1.442279	4.976082
6	1.351526	1.666564	-0.404309
6	0.705040	2.787399	0.144368
6	2.465576	1.869355	-1.232356
6	1.171528	4.075892	-0.113768
1	-0.173641	2.640207	0.768042
6	2.923972	3.162379	-1.501246
1	2.975036	1.018899	-1.675118
6	2.281867	4.267098	-0.940883
1	0.662013	4.931595	0.321855
1	3.785071	3.302687	-2.149732
1	2.639569	5.271582	-1.151390

TS Conc2

ΔE_{gas} -3775.56013848
ΔE_{gas}(ZPE) -3775.248894
ΔG_{gas} -3775.304778

6	-3.542452	1.877848	-0.291730
1	-4.089152	2.000634	-1.220219
1	-4.060651	2.281875	0.571044
1	-2.515451	2.345511	-0.383941
15	0.620332	0.058566	-0.012813
46	-1.576140	0.709816	-0.112586
35	-3.974307	-0.247351	0.042716
6	1.067865	-1.289214	-1.197100
6	0.450619	-1.285213	-2.459007
6	1.981937	-2.309467	-0.893461
6	0.754357	-2.267258	-3.401828
1	-0.279775	-0.513997	-2.692175
6	2.276347	-3.299076	-1.834969
1	2.459457	-2.338313	0.081339
6	1.667090	-3.278172	-3.090681
1	0.268795	-2.250021	-4.373939
1	2.981634	-4.087060	-1.583786
1	1.895938	-4.050084	-3.820650
6	1.143256	-0.610288	1.630387
6	2.423082	-0.411833	2.170481
6	0.203899	-1.352622	2.365729
6	2.756920	-0.949604	3.416206
1	3.159162	0.169286	1.623154
6	0.542868	-1.897434	3.604365
1	-0.797414	-1.491748	1.965794
6	1.820084	-1.695358	4.133425
1	3.750413	-0.783247	3.824614
1	-0.194429	-2.470151	4.160647
1	2.081166	-2.111498	5.102846
6	1.879701	1.372506	-0.357065
6	1.645486	2.656943	0.162045
6	3.042528	1.150081	-1.109566
6	2.559500	3.688318	-0.050561
1	0.736450	2.845435	0.728542
6	3.951124	2.188434	-1.333667
1	3.238532	0.167716	-1.528171
6	3.714529	3.456875	-0.802599
1	2.364919	4.675108	0.361360
1	4.844299	2.002059	-1.924424
1	4.421884	4.262956	-0.978399

Product Conc2

ΔE_{gas} -3775.58977599
ΔE_{gas}(ZPE) -3775.277802
ΔG_{gas} -3775.335800

6	3.097534	-2.592313	-0.136944
1	3.731395	-2.449752	-1.013668
1	3.693432	-2.577254	0.777140
1	2.499427	-3.518322	-0.216421
15	-0.536036	-0.006041	-0.005527
46	1.554823	-1.280351	-0.070808
35	3.258660	0.462388	0.075877
6	-0.724174	1.335717	-1.248897
6	0.118800	1.326332	-2.370782
6	-1.670026	2.364248	-1.110643
6	0.004154	2.317646	-3.347374
1	0.878341	0.555423	-2.465710
6	-1.779462	3.355435	-2.086591
1	-2.312045	2.397354	-0.235086
6	-0.944851	3.331432	-3.207127
1	0.666850	2.303766	-4.208178
1	-2.512138	4.149337	-1.968740
1	-1.027882	4.107575	-3.963196
6	-0.956237	0.781286	1.605522
6	-2.256519	0.801473	2.133927
6	0.087220	1.392630	2.322177
6	-2.510108	1.429025	3.355613
1	-3.070101	0.320764	1.598332
6	-0.174409	2.024938	3.538346
1	1.100239	1.368318	1.928655
6	-1.471160	2.043394	4.057480
1	-3.520021	1.436686	3.757190
1	0.639245	2.495584	4.083378
1	-1.670542	2.530460	5.008271
6	-1.928828	-1.173121	-0.327147
6	-2.009614	-2.326045	0.476994
6	-2.850199	-1.012024	-1.371878
6	-2.996864	-3.284026	0.249993
1	-1.303243	-2.468289	1.292935
6	-3.833740	-1.978320	-1.602190
1	-2.801401	-0.132994	-2.006767
6	-3.911104	-3.112709	-0.793433
1	-3.050266	-4.164478	0.884598
1	-4.540811	-1.839700	-2.415712
1	-4.677378	-3.861278	-0.974925

Adduct Conc1

ΔE_{gas} -3775.58501258

ΔE_{gas}(ZPE) -3775.271469
ΔG_{gas} -3775.328717

6	-4.866702	1.350266	-0.157632
1	-5.947094	1.221813	-0.183968
1	-4.549275	1.945787	0.694554
1	-4.481585	1.748678	-1.092708
15	0.669648	-0.007184	0.004328
46	-1.574004	-0.142521	0.034164
35	-4.083166	-0.458111	0.070767
6	1.501874	-1.117543	-1.222664
6	0.855182	-1.332970	-2.451261
6	2.730806	-1.752048	-0.986259
6	1.432120	-2.146623	-3.426179
1	-0.111555	-0.867710	-2.628844
6	3.301512	-2.577425	-1.959074
1	3.241939	-1.610422	-0.038770
6	2.656746	-2.773385	-3.181221
1	0.919124	-2.301600	-4.371813
1	4.250803	-3.067500	-1.758083
1	3.101382	-3.417005	-3.935770
6	1.519373	-0.422081	1.597210
6	2.685518	0.220063	2.041373
6	0.956859	-1.431403	2.396279
6	3.277354	-0.143467	3.254075
1	3.130117	1.011490	1.445251
6	1.555365	-1.801284	3.600681
1	0.038484	-1.914420	2.071081
6	2.716528	-1.156027	4.033936
1	4.176981	0.367514	3.587691
1	1.108053	-2.584941	4.206628
1	3.177043	-1.436311	4.977691
6	1.351476	1.666119	-0.406260
6	0.704974	2.787577	0.141127
6	2.465481	1.867973	-1.234591
6	1.171410	4.075779	-0.118539
1	-0.173679	2.641092	0.765007
6	2.923824	3.160696	-1.505018
1	2.974953	1.017012	-1.676366
6	2.281706	4.266050	-0.945928
1	0.661889	4.931976	0.316103
1	3.784894	3.300271	-2.153700
1	2.639365	5.270298	-1.157631

TS Conc1

ΔE_{gas} -3775.56211312
ΔE_{gas}(ZPE) -3775.250139
ΔG_{gas} -3775.307659

6	-3.216984	1.631096	-0.398311
1	-4.180315	1.894235	-0.815998
1	-3.006737	2.105241	0.553792
1	-2.414008	1.685696	-1.128562
15	0.616379	-0.047316	0.015834
46	-1.644407	-0.305632	0.087802
35	-4.086571	-0.446599	0.134177
6	1.511229	-1.303615	-1.004005
6	0.818193	-1.899285	-2.070634
6	2.838709	-1.688689	-0.758738
6	1.443441	-2.845382	-2.884206
1	-0.219004	-1.624942	-2.248878
6	3.459704	-2.642178	-1.568198
1	3.386483	-1.253002	0.071549
6	2.765210	-3.219639	-2.633456
1	0.893533	-3.297844	-3.705078
1	4.485972	-2.935584	-1.363102
1	3.249663	-3.963902	-3.259929
6	1.486607	-0.112791	1.646188
6	2.621379	0.656479	1.947368
6	0.980487	-0.986421	2.622875
6	3.238968	0.548043	3.195925
1	3.019922	1.348494	1.211183
6	1.604976	-1.101175	3.865031
1	0.086882	-1.567183	2.406954
6	2.734963	-0.332498	4.154786
1	4.114146	1.153439	3.417331
1	1.201774	-1.781867	4.610045
1	3.215832	-0.414264	5.125932
6	1.159825	1.574039	-0.690719
6	0.604214	2.745013	-0.143653
6	2.050832	1.690585	-1.766689
6	0.943319	3.998813	-0.650235
1	-0.095512	2.669879	0.685775
6	2.379560	2.948508	-2.282332
1	2.488636	0.800578	-2.207354
6	1.830688	4.103574	-1.725818
1	0.510496	4.893437	-0.210229
1	3.068779	3.020778	-3.119660
1	2.088546	5.079762	-2.127478

Product Conc1

ΔE_{gas} -3775.61385808
ΔE_{gas}(ZPE) -3775.300475
ΔG_{gas} -3775.357182

6	-1.619924	1.726486	1.453808
1	-0.609153	2.078174	1.657975
1	-2.122004	1.371364	2.355952
1	-2.214826	2.493258	0.954546
35	-4.107106	-0.019016	0.044339
15	0.611136	0.004799	0.018404
46	-1.670826	0.152095	0.163182
6	0.983961	-1.048105	-1.444206
6	1.804270	-0.629290	-2.501614
6	0.364117	-2.309560	-1.514411
6	2.006492	-1.461543	-3.605683
1	2.283499	0.343948	-2.466854
6	0.571340	-3.136860	-2.617223
1	-0.279678	-2.646640	-0.704806
6	1.392753	-2.713509	-3.665655
1	2.645210	-1.127593	-4.418819
1	0.086620	-4.108075	-2.659638
1	1.550017	-3.356413	-4.527177
6	1.522957	1.578556	-0.253169
6	2.809639	1.812809	0.254024
6	0.888135	2.584169	-1.002430
6	3.452356	3.028391	0.007636
1	3.309022	1.052510	0.846219
6	1.536877	3.793380	-1.253243
1	-0.119412	2.420524	-1.376929
6	2.819623	4.017713	-0.746952
1	4.446911	3.201130	0.409725
1	1.034982	4.563010	-1.832888
1	3.320670	4.963502	-0.933971
6	1.461312	-0.838157	1.415670
6	2.658876	-1.549673	1.232218
6	0.897706	-0.766118	2.699327
6	3.286051	-2.164013	2.317074
1	3.094811	-1.633852	0.240706
6	1.530417	-1.378566	3.782489
1	-0.042898	-0.243922	2.845555
6	2.724695	-2.076414	3.593314
1	4.209904	-2.715061	2.163613
1	1.083519	-1.317992	4.770825
1	3.212556	-2.558846	4.435827

Adduct S_N21

ΔE_{gas} -3775.57049842
ΔE_{gas}(ZPE) -3775.257653
ΔG_{gas} -3775.314848

35	-5.306254	0.119041	0.011545
15	0.856678	-0.031398	0.000986
46	-1.355514	-0.428549	-0.031947
6	1.347344	1.632336	-0.639451
6	0.513011	2.722912	-0.341567
6	2.504230	1.852118	-1.402228
6	0.837102	4.005692	-0.782300
1	-0.397814	2.556259	0.228612
6	2.820711	3.136548	-1.853106
1	3.156543	1.020672	-1.651624
6	1.991266	4.214939	-1.541779
1	0.182048	4.839230	-0.543363
1	3.716899	3.291256	-2.448362
1	2.238227	5.212566	-1.895035
6	1.871572	-1.202717	-1.008633
6	3.116065	-1.698113	-0.591975
6	1.360988	-1.612209	-2.252157
6	3.835335	-2.579426	-1.404131
1	3.524438	-1.403123	0.369745
6	2.086204	-2.480915	-3.066782
1	0.385966	-1.252253	-2.571899
6	3.325183	-2.969467	-2.642885
1	4.795450	-2.959622	-1.064917
1	1.678691	-2.785794	-4.027055
1	3.885607	-3.655457	-3.272446
6	1.641692	-0.102158	1.674418
6	1.158036	-1.051846	2.589647
6	2.689645	0.744428	2.067216
6	1.721008	-1.164781	3.860698
1	0.328777	-1.693364	2.301017
6	3.244494	0.637677	3.345250
1	3.069650	1.493859	1.379419
6	2.764739	-0.317902	4.242367
1	1.336577	-1.905405	4.556987
1	4.051529	1.304369	3.637833
1	3.196290	-0.397740	5.236559
6	-3.739540	-1.068880	-0.072464
1	-4.097146	-2.091561	-0.156573
1	-3.187234	-0.946731	0.876453
1	-3.176635	-0.798773	-0.985485

TS S_N21

ΔE_{gas} -3775.53359853
ΔE_{gas}(ZPE) -3775.221781
ΔG_{gas} -3775.278417

6	1.982080	0.843364	-1.544520
1	1.909363	1.450594	-0.645116
1	2.028481	1.459659	-2.451082
1	2.787647	0.088891	-1.436561
35	4.801161	-0.067239	-0.267636
15	-0.838749	0.011448	-0.045603
46	0.442718	-0.439299	-1.858118
6	-1.908171	-1.467943	0.141769
6	-1.730938	-2.372535	1.200264
6	-2.859477	-1.752716	-0.856643
6	-2.503326	-3.534370	1.264511
1	-0.993500	-2.170577	1.970538
6	-3.629128	-2.912519	-0.783944
1	-3.004505	-1.062740	-1.684598
6	-3.451453	-3.806019	0.276656
1	-2.361066	-4.226479	2.089552
1	-4.365262	-3.119657	-1.555519
1	-4.048896	-4.711648	0.330153
6	0.070765	0.240225	1.524015
6	-0.556415	0.842112	2.630773
6	1.403231	-0.189461	1.630111
6	0.142255	0.995797	3.827037
1	-1.578778	1.200745	2.556472
6	2.098749	-0.022911	2.829545
1	1.930222	-0.620753	0.784369
6	1.468912	0.563916	3.927049
1	-0.346026	1.464295	4.677156
1	3.138873	-0.330080	2.874963
1	2.014037	0.700934	4.856874
6	-1.972436	1.443958	-0.212847
6	-3.270426	1.429517	0.323475
6	-1.508265	2.600873	-0.859901
6	-4.085198	2.558393	0.217728
1	-3.648301	0.538853	0.816345
6	-2.324177	3.727781	-0.956488
1	-0.511562	2.616079	-1.291784
6	-3.613522	3.707901	-0.418988
1	-5.088598	2.537059	0.633808
1	-1.954583	4.617791	-1.457626
1	-4.250280	4.584254	-0.500800

Product S_N21

ΔE_{gas} -3775.61385808
ΔE_{gas}(ZPE) -3775.300475
ΔG_{gas} -3775.357182

6	-1.619924	1.726486	1.453808
1	-0.609153	2.078174	1.657975
1	-2.122004	1.371364	2.355952
1	-2.214826	2.493258	0.954546
35	-4.107106	-0.019016	0.044339
15	0.611136	0.004799	0.018404
46	-1.670826	0.152095	0.163182
6	0.983961	-1.048105	-1.444206
6	1.804270	-0.629290	-2.501614
6	0.364117	-2.309560	-1.514411
6	2.006492	-1.461543	-3.605683
1	2.283499	0.343948	-2.466854
6	0.571340	-3.136860	-2.617223
1	-0.279678	-2.646640	-0.704806
6	1.392753	-2.713509	-3.665655
1	2.645210	-1.127593	-4.418819
1	0.086620	-4.108075	-2.659638
1	1.550017	-3.356413	-4.527177
6	1.522957	1.578556	-0.253169
6	2.809639	1.812809	0.254024
6	0.888135	2.584169	-1.002430
6	3.452356	3.028391	0.007636
1	3.309022	1.052510	0.846219
6	1.536877	3.793380	-1.253243
1	-0.119412	2.420524	-1.376929
6	2.819623	4.017713	-0.746952
1	4.446911	3.201130	0.409725
1	1.034982	4.563010	-1.832888
1	3.320670	4.963502	-0.933971
6	1.461312	-0.838157	1.415670
6	2.658876	-1.549673	1.232218
6	0.897706	-0.766118	2.699327
6	3.286051	-2.164013	2.317074
1	3.094811	-1.633852	0.240706
6	1.530417	-1.378566	3.782489
1	-0.042898	-0.243922	2.845555
6	2.724695	-2.076414	3.593314
1	4.209904	-2.715061	2.163613
1	1.083519	-1.317992	4.770825
1	3.212556	-2.558846	4.435827

Adduct S_N22

ΔE_{gas} -3775.57047904
ΔE_{gas}(ZPE) -3775.257548
ΔG_{gas} -3775.317394

6	3.739000	-1.047341	-0.191320
1	4.092309	-2.056254	-0.386386
1	3.187657	-1.025876	0.765561
1	3.177216	-0.676993	-1.069098
35	5.311271	0.118030	0.019315
15	-0.858437	-0.029394	-0.005163
46	1.355184	-0.413788	-0.085318
6	-1.333385	1.754212	-0.118257
6	-2.467784	2.205469	-0.809581
6	-0.508745	2.695419	0.520819
6	-2.772393	3.568678	-0.855426
1	-3.110993	1.495054	-1.320027
6	-0.821249	4.054013	0.483952
1	0.386188	2.355729	1.036761
6	-1.953335	4.494097	-0.206906
1	-3.651056	3.904753	-1.399884
1	-0.173862	4.769705	0.983588
1	-2.190949	5.553853	-0.245596
6	-1.838737	-0.827833	-1.355577
6	-3.108023	-1.390895	-1.155096
6	-1.274021	-0.870400	-2.641501
6	-3.798098	-1.978345	-2.219115
1	-3.558255	-1.379075	-0.167226
6	-1.969437	-1.445843	-3.704448
1	-0.280307	-0.458404	-2.800114
6	-3.233230	-2.004307	-3.494824
1	-4.778065	-2.415971	-2.047118
1	-1.519584	-1.468815	-4.693502
1	-3.770847	-2.462968	-4.320426
6	-1.694900	-0.606083	1.540775
6	-2.753073	0.087705	2.147453
6	-1.240045	-1.797985	2.128964
6	-3.346065	-0.404884	3.313110
1	-3.111277	1.017593	1.716020
6	-1.840980	-2.294237	3.285530
1	-0.403192	-2.326429	1.678551
6	-2.894758	-1.596855	3.881843
1	-4.160754	0.146335	3.775539
1	-1.478725	-3.218536	3.727778
1	-3.356335	-1.977104	4.789257

TS S_N22

ΔE_{gas} -3775.50786776
ΔE_{gas}(ZPE) -3775.198819
ΔG_{gas} -3775.258115

6	2.831173	-1.790480	-1.779120
1	3.001500	-1.585507	-2.840403
1	3.001461	-2.844266	-1.538693
1	3.323673	-1.066603	-1.075362
35	4.757056	0.106599	0.134933
46	1.045167	-1.103031	-1.110126
15	-0.881090	-0.048886	-0.060830
6	-2.383637	0.122713	-1.113861
6	-2.202761	0.448809	-2.468843
6	-3.686172	-0.062210	-0.626891
6	-3.300917	0.598894	-3.315157
1	-1.197851	0.590191	-2.861606
6	-4.784331	0.080867	-1.478774
1	-3.844621	-0.324056	0.414946
6	-4.594636	0.412772	-2.821142
1	-3.146141	0.853882	-4.359885
1	-5.788186	-0.068013	-1.090292
1	-5.450354	0.521948	-3.481627
6	-1.460282	-0.944050	1.440609
6	-1.762422	-0.296222	2.646790
6	-1.571825	-2.343472	1.370860
6	-2.173077	-1.035239	3.759393
1	-1.668719	0.782588	2.721449
6	-1.991736	-3.077352	2.479364
1	-1.329156	-2.860829	0.444711
6	-2.290871	-2.423299	3.677614
1	-2.397584	-0.522554	4.690695
1	-2.074769	-4.158500	2.411332
1	-2.607329	-2.995372	4.545334
6	-0.489326	1.659261	0.495581
6	0.843751	1.959091	0.823847
6	-1.465146	2.664557	0.594448
6	1.190055	3.239999	1.256992
1	1.621518	1.203400	0.734594
6	-1.112219	3.944979	1.023544
1	-2.496075	2.452176	0.325919
6	0.213682	4.232996	1.357112
1	2.225553	3.457401	1.501920
1	-1.872972	4.717963	1.092313
1	0.485935	5.232192	1.686067

Product S_N22

ΔE_{gas} -3775.58977464
ΔE_{gas}(ZPE) -3775.277804
ΔG_{gas} -3775.335820

35	-3.258870	0.463136	0.076138
46	-1.555070	-1.279683	-0.068944
15	0.535951	-0.005762	-0.005386
6	1.927863	-1.174450	-0.325128
6	2.008785	-2.325367	0.481864
6	2.848218	-1.016574	-1.371241
6	2.995240	-3.284501	0.256260
1	1.303191	-2.465109	1.298905
6	3.830948	-1.984030	-1.600127
1	2.799268	-0.139113	-2.008279
6	3.908495	-3.116394	-0.788553
1	3.048780	-4.163359	0.893060
1	4.537239	-1.847901	-2.414748
1	4.674134	-3.865881	-0.968931
6	0.724923	1.333747	-1.251084
6	1.671559	2.361819	-1.114909
6	-0.118427	1.323052	-2.372690
6	1.781390	3.351237	-2.092612
1	2.313898	2.396030	-0.239629
6	-0.003371	2.312579	-3.351042
1	-0.878577	0.552545	-2.466029
6	0.946420	3.325915	-3.212847
1	2.514673	4.144812	-1.976340
1	-0.666355	2.297698	-4.211607
1	1.029789	4.100686	-3.970284
6	0.956851	0.784005	1.604281
6	-0.086280	1.396492	2.320408
6	2.257373	0.805026	2.132083
6	0.175892	2.030763	3.535452
1	-1.099505	1.371482	1.927448
6	2.511508	1.434558	3.352630
1	3.070703	0.323380	1.596943
6	1.472871	2.050080	4.053962
1	-0.637530	2.502254	4.080099
1	3.521597	1.442850	3.753754
1	1.672682	2.538682	5.003874
6	-3.097728	-2.591822	-0.134396
1	-2.499618	-3.517976	-0.211782
1	-3.694522	-2.575223	0.779066
1	-3.730654	-2.450542	-1.011999

2.2.2 Species Optimized in THF

2.2.2.1 PF_3

$PdPF_3$

ΔE_{THF} -768.948805749
ΔE_{THF}(ZPE) -768.939683
ΔG_{THF} -768.970230

46	0.000000	0.000000	1.263491
15	0.000000	0.000000	-0.835311
9	0.000000	1.381897	-1.688552
9	-1.196758	-0.690949	-1.688552
9	1.196758	-0.690949	-1.688552

PF_3

ΔE_{THF} -640.986182172
ΔE_{THF}(ZPE) -640.978317
ΔG_{THF} -641.004579

15	0.000000	0.000000	0.523569
9	0.000000	1.395059	-0.290872
9	1.208157	-0.697530	-0.290872
9	-1.208157	-0.697530	-0.290872

Adduct Conc2

ΔE_{THF} -3380.29377687
ΔE_{THF}(ZPE) -3380.246469
ΔG_{THF} -3380.288598

15	-2.186814	0.051122	0.000281
46	-0.064660	-0.048806	-0.001010
35	2.509202	-0.418929	0.000324
6	3.265852	1.421463	0.001006
1	2.927926	1.899817	0.915719
1	4.345288	1.296139	-0.023136
1	2.889898	1.916281	-0.889785
9	-3.068442	-0.653761	-1.161508
9	-3.061214	-0.541420	1.228682
9	-2.959643	1.472930	-0.064723

TS Conc2

ΔE_{THF} -3380.26066761
ΔE_{THF}(ZPE) -3380.215385
ΔG_{THF} -3380.252637

15	-2.003385	-0.143430	-0.000534
46	0.101442	0.499390	0.000565
35	2.342530	-0.721492	-0.000274
6	2.049794	1.561982	-0.001746
1	2.611604	1.731633	0.908798
1	2.610228	1.730091	-0.913404
1	1.095995	2.167393	-0.001518
9	-2.538108	-1.167379	-1.120769
9	-2.610706	-0.924552	1.268651
9	-3.209043	0.917565	-0.146970

Product Conc2

ΔE_{THF} -3380.28551540
ΔE_{THF}(ZPE) -3380.239912
ΔG_{THF} -3380.279586

15	-1.774662	0.045864	-0.000100
46	0.409652	-0.889215	-0.000280
35	1.535084	1.302217	0.000002
6	2.263773	-1.692826	0.000550
1	2.815878	-1.425087	-0.900590
1	2.814485	-1.425760	0.902747
1	1.950633	-2.749092	-0.000110
9	-3.090020	-0.869432	-0.000858
9	-2.183776	1.013434	-1.202283
9	-2.183499	1.011021	1.204137

Adduct Conc1

ΔE_{THF} -3380.29375935
ΔE_{THF}(ZPE) -3380.246441
ΔG_{THF} -3380.288460

6	3.270455	1.419745	0.002107
1	2.907647	1.910837	0.900431
1	4.349844	1.291566	0.010899
1	2.921515	1.903812	-0.905479
15	-2.187557	0.052356	0.001596
46	-0.065213	-0.046739	-0.006765
35	2.509884	-0.419025	0.003674
9	-3.087192	-1.220684	-0.436197
9	-2.989889	1.126559	-0.907976
9	-3.015642	0.361442	1.359745

TS Conc1

ΔE_{THF} -3380.26267971
ΔE_{THF}(ZPE) -3380.217031
ΔG_{THF} -3380.255113

6	-1.451080	1.886921	-0.001176
1	-0.889686	2.072162	-0.911655
1	-2.464995	2.259159	-0.030924
1	-0.939690	2.075486	0.937376
15	2.045159	-0.020087	-0.000037
46	-0.119770	-0.217070	-0.002862
35	-2.557662	-0.258297	0.002138
9	2.962586	-0.933998	-0.958083
9	2.895091	-0.273011	1.345411
9	2.736886	1.384630	-0.379590

Product Conc1

ΔE_{THF} -3380.30498561
ΔE_{THF} (ZPE) -3380.257940
ΔG_{THF} -3380.297855

46	0.222316	-0.091818	0.000357
15	-2.006108	-0.147639	-0.000137
6	0.172137	1.960574	-0.000890
1	-0.370596	2.275232	0.891824
1	1.212444	2.274950	0.025705
1	-0.323312	2.265210	-0.924016
35	2.666058	-0.204306	0.000354
9	-2.821479	0.637589	-1.118152
9	-2.814022	0.379545	1.265819
9	-2.697643	-1.571570	-0.149326

Adduct S_N21

ΔE_{THF} -3380.27795099
ΔE_{THF} (ZPE) -3380.230961
ΔG_{THF} -3380.273659

6	-2.243962	0.227805	-0.079767
1	-1.953793	0.799244	-0.957557
1	-1.869758	0.680884	0.834505
1	-1.944939	-0.814839	-0.163047
35	-4.219729	0.259785	0.014913
15	2.380934	0.556128	0.003016
46	1.164165	-1.155866	0.001982
9	3.725071	0.641256	-0.902847
9	3.089773	1.093815	1.360553
9	1.813735	2.009745	-0.445894

TS S_N21

ΔE_{THF} -3380.25317856
ΔE_{THF}(ZPE) -3380.207229
ΔG_{THF} -3380.248099

6	-1.056152	-0.180492	0.005781
1	-1.009483	0.586810	-0.754409
1	-1.123835	0.140559	1.037991
1	-1.478066	-1.148005	-0.270520
35	-3.668181	0.373962	-0.000844
15	2.073952	0.603152	-0.000428
46	0.846338	-1.183552	0.001796
9	3.511134	0.556464	-0.700725
9	2.540350	1.260875	1.380930
9	1.536714	1.939442	-0.690695

Product S_N21

ΔE_{THF} -3380.25326647
ΔE_{THF}(ZPE) -3380.206902
ΔG_{THF} -3380.248892

6	-0.980203	-0.219104	0.004237
1	-0.981964	0.543657	-0.764396
1	-1.091147	0.130176	1.025268
1	-1.455857	-1.169119	-0.252468
35	-3.710604	0.365107	-0.000614
15	2.064236	0.630815	-0.000751
46	0.887253	-1.196341	0.001898
9	3.520592	0.591374	-0.651786
9	2.464156	1.321648	1.380780
9	1.515714	1.931490	-0.738817

Adduct S_N22

ΔE_{THF} -3380.27717051
ΔE_{THF}(ZPE) -3380.230321
ΔG_{THF} -3380.268728

6	-2.725526	0.079129	0.188101
1	-2.462502	-0.878327	0.631328
1	-2.286476	0.194350	-0.800713
1	-2.462935	0.909537	0.839746
35	-4.686481	0.105694	-0.036648
46	0.897078	-0.322946	-0.005766
15	2.949636	0.131530	-0.007574
9	3.748690	0.445971	1.370110
9	4.052700	-0.914777	-0.574155
9	3.541030	1.411355	-0.811228

TS S_N22

ΔE_{THF} -3380.24309739
ΔE_{THF}(ZPE) -3380.198896
ΔG_{THF} -3380.238525

6	-1.630309	-0.092188	-0.034419
1	-1.626572	0.917474	-0.442647
1	-1.673668	-0.228535	1.043832
1	-1.705115	-0.955997	-0.691402
35	-4.164597	0.066558	0.006770
46	0.506362	-0.118499	-0.000905
15	2.747123	0.044764	0.008227
9	3.615035	-0.609159	-1.176166
9	3.426205	1.501345	-0.050542
9	3.630824	-0.528835	1.224261

2.2.2.2 PH_3

$PdPH_3$

ΔE_{THF} -471.094235110
ΔE_{THF}(ZPE) -471.067408
ΔG_{THF} -471.094240

46	0.646521	0.000000	-0.000002
15	-1.530983	0.000009	-0.000034
1	-2.258519	1.184401	-0.287218
1	-2.258619	-0.841206	-0.881693
1	-2.258099	-0.343315	1.169491

PH_3

ΔE_{THF} -343.145737790
ΔE_{THF}(ZPE) -343.121699
ΔG_{THF} -343.142740

15	-0.000001	-0.000003	-0.126417
1	0.387064	1.138604	0.632067
1	-1.179580	-0.234079	0.632098
1	0.792532	-0.904478	0.632098

Adduct Conc2

ΔE_{THF} -3082.44242094
ΔE_{THF}(ZPE) -3082.377373
ΔG_{THF} -3082.415159

15	-2.919336	0.167098	0.000001
46	-0.710142	-0.037146	0.000000
35	1.803885	-0.422095	0.000000
1	-3.516248	1.452983	-0.000481
1	-3.699023	-0.368173	-1.056107
1	-3.698982	-0.367356	1.056555
6	2.647887	1.380064	0.000000
1	3.721706	1.208816	-0.000019
1	2.312887	1.884458	-0.901956
1	2.312912	1.884446	0.901974

TS Conc2

ΔE_{THF} -3082.41571724
ΔE_{THF}(ZPE) -3082.352922
ΔG_{THF} -3082.389081

15	-2.736824	-0.414248	0.000032
46	-0.563482	0.262058	-0.000003
35	1.868642	-0.552232	-0.000006
1	-3.794828	0.527722	0.000005
1	-3.229393	-1.213452	-1.059017
1	-3.229379	-1.213377	1.059144
6	1.314252	1.603012	-0.000031
1	1.835497	1.877152	0.909572
1	1.835511	1.877128	-0.909634
1	0.267123	2.013911	-0.000047

Product Conc2

ΔE_{THF} -3082.45217364
ΔE_{THF}(ZPE) -3082.388849
ΔG_{THF} -3082.425219

15	-2.288217	-0.864900	-0.000014
46	-0.375333	0.690362	0.000018
35	1.425915	-0.988539	-0.000002
1	-3.623061	-0.397533	-0.001080
1	-2.404344	-1.784636	-1.064969
1	-2.405626	-1.783379	1.065892
6	1.060132	2.108802	-0.000047
1	1.677162	2.069540	0.899833
1	1.678798	2.068487	-0.898739
1	0.397827	2.990438	-0.001186

Adduct Conc1

ΔE_{THF} -3082.44233480
ΔE_{THF}(ZPE) -3082.377237
ΔG_{THF} -3082.414385

15	2.916948	0.172562	0.000153
46	0.710787	-0.041983	0.000247
35	-1.805531	-0.420975	-0.000212
1	3.514543	1.400186	-0.383901
1	3.668283	-0.000375	1.191294
1	3.724950	-0.658854	-0.817475
6	-2.640290	1.387756	-0.000569
1	-3.696936	1.228853	-0.201918
1	-2.469006	1.807460	0.987439
1	-2.156935	1.973116	-0.778237

TS Conc1

ΔE_{THF} -3082.41690771
ΔE_{THF} (ZPE) -3082.353831
ΔG_{THF} -3082.391603

6	1.027780	1.847402	0.000011
1	0.495365	2.063127	0.921174
1	2.048855	2.203923	-0.001225
1	0.493248	2.063111	-0.919941
15	-2.783925	0.003661	0.000013
46	-0.525184	-0.144790	-0.000009
35	1.920109	-0.312271	0.000004
1	-3.465466	0.655091	-1.056208
1	-3.465962	0.646312	1.061285
1	-3.559211	-1.181041	-0.005071

Product Conc1

ΔE_{THF} -3082.47471071
ΔE_{THF}(ZPE) -3082.410227
ΔG_{THF} -3082.444925

46	-0.386812	-0.145217	-0.000086
15	-2.669207	-0.353312	0.000092
1	-3.400611	0.208946	-1.065129
1	-3.177190	-1.668690	-0.022020
1	-3.395919	0.170567	1.087896
6	-0.621804	1.873959	0.000029
1	-1.171505	2.157675	0.900362
1	0.387108	2.283468	0.005884
1	-1.161111	2.157328	-0.906681
35	2.099471	-0.130669	0.000059

Adduct S_N21

ΔE_{THF} -3082.42432508
ΔE_{THF}(ZPE) -3082.359977
ΔG_{THF} -3082.398244

6	-1.573061	0.206048	-0.000114
1	-1.271996	0.726472	-0.905046
1	-1.272565	0.745387	0.893864
1	-1.217149	-0.821389	0.010853
35	-3.555820	0.128188	0.000017
15	3.069530	1.129680	-0.000019
1	4.059514	1.289435	-1.003655
1	2.538556	2.441696	-0.097882
1	3.923732	1.391888	1.101969
46	1.762805	-0.618295	0.000006

TS S_N21

ΔE_{THF} -3082.41310317
ΔE_{THF}(ZPE) -3082.349888
ΔG_{THF} -3082.386986

6	-0.757274	0.065607	0.002087
1	-0.664184	0.609698	-0.924912
1	-0.666638	0.598071	0.936086
1	-0.805333	-1.021962	-0.004833
35	-3.112946	0.176912	-0.000288
15	2.650951	1.215347	-0.000226
1	3.649001	1.406531	-0.984936
1	2.004764	2.464938	-0.142105
1	3.441618	1.539801	1.127431
46	1.451592	-0.661149	-0.000126

Product S_N21

ΔE_{THF} -3082.42779471
ΔE_{THF}(ZPE) -3082.363748
ΔG_{THF} -3082.402900

6	0.151835	-0.114896	0.055459
1	0.389905	0.275790	1.044932
1	0.417431	0.583904	-0.735251
1	0.581185	-1.110304	-0.117322
35	3.536232	0.111134	-0.005711
15	-2.420764	1.469650	-0.003410
1	-3.813739	1.674846	0.023225
1	-1.997378	2.281328	1.064523
1	-2.043104	2.257775	-1.105116
46	-1.780478	-0.678444	-0.005581

Adduct S_N22

ΔE_{THF} -3082.42597622
ΔE_{THF}(ZPE) -3082.361941
ΔG_{THF} -3082.398761

6	-1.292672	0.920419	-0.005076
1	-0.738317	0.711444	-0.935408
1	-1.642543	1.948984	-0.014800
1	-0.744527	0.727277	0.931943
35	-2.870968	-0.260070	-0.000263
46	1.099732	0.148830	0.002758
15	3.260501	-0.342708	-0.003141
1	4.164359	0.412256	-0.789605
1	4.011027	-0.303993	1.197399
1	3.694713	-1.621617	-0.429623

TS S_N22

ΔE_{THF} -3082.40189455
ΔE_{THF}(ZPE) -3082.340316
ΔG_{THF} -3082.375763

6	-0.804832	-0.051008	-0.002665
1	-0.911675	1.030705	-0.078073
1	-0.929298	-0.526258	0.969215
1	-0.935340	-0.655728	-0.898562
35	-3.399514	0.017605	0.000377
46	1.272532	-0.020046	0.000146
15	3.662386	0.039165	0.000429
1	4.342789	1.114165	-0.617345
1	4.372764	0.063885	1.222912
1	4.400509	-1.002244	-0.608483

Product S_N22

ΔE_{THF} -3082.40226540
ΔE_{THF}(ZPE) -3082.340200
ΔG_{THF} -3082.379398

6	0.698370	-0.038850	-0.000238
1	0.914118	1.005915	-0.233937
1	0.929719	-0.760502	-0.785842
1	0.925668	-0.356823	1.019042
35	3.550537	0.018960	0.000169
46	-1.329147	-0.028471	-0.000280
15	-3.777060	0.050484	0.000438
1	-4.430618	1.266928	-0.297277
1	-4.510992	-0.775018	-0.880304
1	-4.490231	-0.258591	1.180178

2.2.2.3 $P(CH_3)_3$

PdP(CH3)3

ΔE$_{THF}$ -589.071169041
ΔE$_{THF}$(ZPE) -588.957112
ΔG$_{THF}$ -588.990756

46	-1.325507	-0.000054	0.000225
15	0.873337	0.000280	-0.000267
6	1.719958	-0.292595	1.625199
1	1.418385	-1.264598	2.025402
1	2.810544	-0.273215	1.510026
1	1.420424	0.480230	2.338591
6	1.718250	1.555045	-0.559846
1	1.417339	2.386913	0.083119
1	2.808843	1.446221	-0.520976
1	1.416789	1.787412	-1.585070
6	1.718160	-1.262567	-1.066134
1	1.416583	-1.123638	-2.108054
1	2.808819	-1.174115	-0.991904
1	1.417347	-2.266239	-0.752801

P(CH3)3

ΔE$_{THF}$ -461.115521684
ΔE$_{THF}$(ZPE) -461.003103
ΔG$_{THF}$ -461.032490

15	0.000438	-0.000547	-0.595742
6	1.564144	-0.517510	0.276266
1	1.828260	-1.537807	-0.020107
1	2.385005	0.142014	-0.023283
1	1.460417	-0.481024	1.367545
6	-0.333695	1.613002	0.275480
1	0.417391	2.352168	-0.021343
1	-1.315739	1.994022	-0.022760
1	-0.312344	1.505194	1.366802
6	-1.230989	-1.094804	0.275897
1	-2.245936	-0.813618	-0.023149
1	-1.070162	-2.136300	-0.020676
1	-1.150227	-1.020568	1.367235

Adduct Conc2

ΔE$_{THF}$ -3200.41954967
ΔE$_{THF}$ (ZPE) -3200.267386
ΔG$_{THF}$ -3200.311690

15	2.243644	0.064291	0.000756
46	0.001481	-0.074730	-0.000862
35	-2.511839	-0.403934	0.000775
6	-3.341968	1.405808	0.000535
1	-3.000601	1.908709	-0.899950
1	-4.417437	1.244829	-0.001786
1	-3.004261	1.907055	0.903329
6	3.050186	0.733672	1.530988
1	4.141227	0.757779	1.425355
1	2.685913	1.746911	1.722914
1	2.785745	0.107042	2.387487
6	3.173082	-1.523773	-0.227312
1	4.256028	-1.352938	-0.218262
1	2.911901	-2.218019	0.576291
1	2.889317	-1.980192	-1.179732
6	3.023344	1.126916	-1.304017
1	2.661935	2.154261	-1.203118
1	4.116372	1.120295	-1.218856
1	2.737597	0.759437	-2.293637

TS Conc2

ΔE$_{THF}$ -3200.39405341
ΔE$_{THF}$(ZPE) -3200.243792
ΔG$_{THF}$ -3200.285321

15	2.113679	-0.125665	-0.000272
46	-0.118239	0.394476	0.000827
35	-2.495893	-0.630062	-0.000412
6	-2.130985	1.542657	-0.001889
1	-2.667995	1.785744	-0.911603
1	-2.671344	1.787190	0.905465
1	-1.112982	2.029460	-0.000157
6	3.317269	1.274535	-0.168370
1	4.351193	0.910779	-0.160258
1	3.131378	1.806153	-1.105949
1	3.177381	1.977299	0.657940
6	2.759362	-0.980562	1.510548
1	3.829488	-1.196712	1.414464
1	2.598412	-0.347225	2.387479
1	2.215095	-1.917334	1.659544
6	2.693474	-1.263463	-1.342425
1	2.483994	-0.815595	-2.317957
1	3.769199	-1.456416	-1.258937
1	2.151529	-2.211065	-1.276758

Product Conc2

ΔE$_{THF}$ -3200.43296615
ΔE$_{THF}$(ZPE) -3200.282392
ΔG$_{THF}$ -3200.324392

15	1.833003	-0.098177	-0.000152
46	-0.413895	0.867827	-0.000296
35	-1.668468	-1.253210	0.000023
6	-2.201152	1.837710	0.000324
1	-2.793750	1.626140	-0.892927
1	-2.784417	1.636352	0.902143
1	-1.823387	2.874425	-0.007671
6	2.232609	-1.177472	1.443345
1	3.243722	-1.589955	1.360938
1	2.155474	-0.597009	2.367231
1	1.510049	-1.996624	1.490468
6	2.233419	-1.180048	-1.441459
1	2.157564	-0.601080	-2.366389
1	3.244201	-1.592997	-1.357325
1	1.510416	-1.998840	-1.487930
6	3.232588	1.112510	-0.000713
1	4.200422	0.599829	-0.000251
1	3.167862	1.748765	-0.888223
1	3.167558	1.749746	0.886071

Adduct Conc1

ΔE$_{THF}$ -3200.41962993
ΔE$_{THF}$(ZPE) -3200.267350
ΔG$_{THF}$ -3200.311080

15	2.243873	0.060920	0.000073
46	0.001418	-0.072327	0.000940
35	-2.510014	-0.406017	-0.000185
6	-3.348991	1.399884	-0.000572
1	-3.006613	1.905986	-0.898893
1	-4.423641	1.233637	-0.007446
1	-3.017421	1.901290	0.904421
6	2.976012	1.764528	-0.037750
1	4.071705	1.724867	-0.035637
1	2.637753	2.288011	-0.936467
1	2.636032	2.328496	0.835491
6	3.135623	-0.678455	1.448212
1	4.220647	-0.556947	1.348295
1	2.802633	-0.192279	2.369562
1	2.898771	-1.743814	1.518717
6	3.135223	-0.742680	-1.413787
1	2.807035	-0.292854	-2.355105
1	4.220746	-0.623518	-1.316498
1	2.892305	-1.808664	-1.440918

TS Conc1

ΔE$_{THF}$ -3200.39564957
ΔE$_{THF}$(ZPE) -3200.245247
ΔG$_{THF}$ -3200.288252

6	1.742547	1.848256	0.002449
1	1.266366	2.064174	0.953091
1	2.762165	2.203606	-0.064655
1	1.150680	2.064256	-0.881385
15	-2.129594	-0.007242	0.000816
46	0.146634	-0.161576	-0.000501
35	2.596197	-0.313685	0.000382
6	-3.044280	-1.549303	-0.465898
1	-2.753505	-1.856649	-1.474357
1	-2.781473	-2.353665	0.226956
1	-4.128199	-1.389345	-0.436597
6	-2.941295	0.428066	1.608008
1	-4.031791	0.461561	1.503840
1	-2.675465	-0.315820	2.364362
1	-2.583108	1.404335	1.947059
6	-2.889065	1.234521	-1.144622
1	-2.586873	1.015596	-2.172666
1	-3.982873	1.216720	-1.079765
1	-2.531516	2.236078	-0.888067

Product Conc1

ΔE$_{THF}$ -3200.46191612
ΔE$_{THF}$(ZPE) -3200.310004
ΔG$_{THF}$ -3200.351540

46	0.236811	-0.018633	-0.000470
15	-2.044880	-0.160783	-0.000523
6	0.095009	2.006174	0.001422
1	-0.569232	2.347783	0.798453
1	1.113276	2.359259	0.167998
1	-0.273106	2.318806	-0.979062
35	2.738573	-0.230470	0.000795
6	-2.963903	0.792052	-1.276816
1	-4.035744	0.580050	-1.210805
1	-2.802835	1.862758	-1.128060
1	-2.600990	0.518280	-2.270756
6	-2.889379	0.281636	1.573784
1	-2.721798	1.337631	1.801397
1	-3.966053	0.098606	1.494832
1	-2.478754	-0.319463	2.389054
6	-2.544028	-1.909177	-0.296895
1	-2.110771	-2.551642	0.474408
1	-3.634355	-2.004478	-0.271953
1	-2.175989	-2.236377	-1.272835

Adduct S_N21

ΔE$_{THF}$ -3200.40170754
ΔE$_{THF}$ (ZPE) -3200.249886
ΔG$_{THF}$ -3200.295338

6	2.258050	0.104213	-0.259737
1	1.792371	-0.086589	0.703894
1	1.909041	1.036167	-0.696585
1	2.126139	-0.731396	-0.942311
35	4.210087	0.300859	0.047599
15	-2.471801	0.529960	0.006748
46	-1.016081	-1.123479	0.010638
6	-1.845687	2.222866	-0.419899
1	-1.406330	2.210635	-1.421110
1	-2.656773	2.960013	-0.392323
1	-1.069421	2.517721	0.291622
6	-3.350720	0.871989	1.604803
1	-2.619496	1.117324	2.380059
1	-4.052730	1.707324	1.494514
1	-3.899453	-0.019902	1.920302
6	-3.907467	0.378779	-1.158995
1	-4.570623	1.248441	-1.078539
1	-3.539671	0.300856	-2.185625
1	-4.474390	-0.527114	-0.927465

TS S_N21

ΔE$_{THF}$ -3200.39373608
ΔE$_{THF}$(ZPE) -3200.242863
ΔG$_{THF}$ -3200.286047

6	1.438515	-0.115113	-0.014109
1	1.248193	0.178568	1.006984
1	1.172323	0.563772	-0.808224
1	1.600063	-1.161374	-0.250439
35	3.684106	0.385566	0.001842
15	-2.180728	0.555035	-0.001788
46	-0.753963	-1.166277	0.000527
6	-1.481081	2.230771	-0.351892
1	-1.017599	2.239235	-1.342248
1	-2.267433	2.993137	-0.318011
1	-0.716028	2.474029	0.390538
6	-3.091496	0.849401	1.582591
1	-2.376722	1.047046	2.385911
1	-3.771155	1.703929	1.486577
1	-3.668454	-0.041489	1.845140
6	-3.568319	0.457668	-1.223386
1	-4.224618	1.330996	-1.134481
1	-3.162728	0.413731	-2.237728
1	-4.152049	-0.449538	-1.045123

Product S_N21

ΔE_{THF} -3200.41951992
ΔE_{THF} (ZPE) -3200.267742
ΔG_{THF} -3200.311680

6	0.600289	-0.256065	0.205580
1	0.653713	0.265618	1.162762
1	0.812513	0.413957	-0.627830
1	1.281987	-1.114627	0.187556
35	4.343871	0.278149	-0.020858
15	-2.235688	0.738527	-0.008299
46	-1.146633	-1.223295	-0.018053
6	-1.827019	1.887565	-1.377573
1	-1.996950	1.391400	-2.335194
1	-2.463728	2.774436	-1.311604
1	-0.779652	2.192172	-1.316233
6	-2.064261	1.738302	1.521475
1	-1.027711	2.061676	1.640385
1	-2.710870	2.618885	1.457603
1	-2.350162	1.141265	2.390771
6	-4.037461	0.409333	-0.173161
1	-4.579424	1.360954	-0.214536
1	-4.231456	-0.152871	-1.090205
1	-4.392607	-0.169204	0.683521

Adduct S_N22

ΔE_{THF} -3200.40427319
ΔE_{THF} (ZPE) -3200.252617
ΔG_{THF} -3200.296388

6	2.082420	0.941792	0.004615
1	1.518459	0.774990	-0.929961
1	1.519957	0.770449	0.938848
1	2.493972	1.947257	0.006403
35	3.590794	-0.330653	-0.000079
46	-0.317499	0.288270	-0.001909
15	-2.516310	-0.145717	0.000585
6	-3.139850	-1.273141	-1.330945
1	-4.222025	-1.423862	-1.241584
1	-2.916506	-0.841556	-2.310543
1	-2.634771	-2.240271	-1.258314
6	-3.199369	-0.959861	1.518163
1	-4.276986	-1.134550	1.418494
1	-2.693708	-1.916005	1.678962
1	-3.016963	-0.324065	2.388941
6	-3.654309	1.304178	-0.183084
1	-4.702287	0.982725	-0.172084
1	-3.485397	2.008412	0.636179
1	-3.445291	1.816865	-1.126014

TS S_N22

ΔE_{THF} -3200.38017414
ΔE_{THF} (ZPE) -3200.231579
ΔG_{THF} -3200.274212

6	-1.661897	-0.063330	-0.037616
1	-1.735326	0.943340	-0.447218
1	-1.734821	-0.214052	1.038269
1	-1.772186	-0.918172	-0.701564
35	-4.196562	0.018921	0.016313
46	0.432125	-0.018649	-0.022825
15	2.821683	0.013077	0.010533
6	3.633126	1.632354	-0.373830
1	4.724549	1.548878	-0.327782
1	3.341605	1.959152	-1.376105
1	3.300471	2.388212	0.343335
6	3.628549	-0.442089	1.613959
1	4.720069	-0.384778	1.537628
1	3.288308	0.236080	2.401798
1	3.342265	-1.460953	1.890131
6	3.678471	-1.127781	-1.169898
1	4.765127	-0.991929	-1.132400
1	3.439180	-2.163746	-0.912491
1	3.327928	-0.937453	-2.188273

Product S_N22

ΔE_{THF} -3200.38193964
ΔE_{THF} (ZPE) -3200.232623
ΔG_{THF} -3200.271792

6	1.511426	-0.020586	-0.001429
1	1.770863	-0.452914	0.968328
1	1.762413	1.037658	-0.108663
1	1.771414	-0.642126	-0.861638
35	4.492295	0.010580	0.001361
46	-0.507467	-0.018085	-0.002826
15	-2.977648	0.008340	0.000684
6	-3.789545	-0.554964	1.562657
1	-4.880298	-0.511845	1.478253
1	-3.488390	-1.583456	1.779868
1	-3.470105	0.078508	2.395179
6	-3.763087	1.657884	-0.280990
1	-4.855557	1.584969	-0.260396
1	-3.438843	2.356239	0.495198
1	-3.448453	2.051229	-1.251431
6	-3.802174	-1.047179	-1.273018
1	-4.892645	-0.977108	-1.197931
1	-3.490267	-0.725412	-2.270793
1	-3.501964	-2.090155	-1.137200

2.2.2.4 PPh_3

$PdPPh_3$

ΔE_{THF} -1164.24523102
ΔE_{THF}(ZPE) -1163.969857
ΔG_{THF} -1164.019742

15	0.000594	-0.001531	0.364628
6	-0.381411	1.638042	-0.412666
6	1.598919	-0.489388	-0.440208
6	-1.231924	-1.138358	-0.425752
6	-2.486625	-1.281670	0.191579
6	-3.462987	-2.110664	-0.361767
6	-3.193747	-2.824808	-1.533343
6	-1.947412	-2.698469	-2.149739
6	-0.973223	-1.857437	-1.603193
1	-2.687770	-0.744813	1.116054
1	-4.428680	-2.207833	0.127022
1	-3.949210	-3.479291	-1.959398
1	-1.729492	-3.253024	-3.058639
1	-0.010242	-1.765425	-2.095990
6	2.087763	0.109832	-1.611411
6	3.302987	-0.303525	-2.166346
6	4.040202	-1.324841	-1.564329
6	3.560654	-1.930948	-0.399038
6	2.355099	-1.509850	0.162361
1	1.522791	0.901448	-2.093758
1	3.670642	0.174891	-3.070254
1	4.984859	-1.643715	-1.996231
1	4.131091	-2.722775	0.079030
1	1.995950	-1.965586	1.082442
6	0.131313	2.793535	0.201776
6	-0.104610	4.056040	-0.343478
6	-0.873484	4.185240	-1.503825
6	-1.397817	3.045675	-2.116977
6	-1.151055	1.779205	-1.578531
1	0.710642	2.695027	1.117162
1	0.301782	4.938574	0.143279
1	-1.067064	5.168609	-1.923543
1	-2.000051	3.138304	-3.016878
1	-1.563496	0.902353	-2.068192
46	0.018989	-0.020422	2.566909

PPh_3

ΔE_{THF} -1036.28930268
ΔE_{THF}(ZPE) -1036.015022
ΔG_{THF} -1036.061217

15	-0.000399	-0.001583	-1.198073
6	0.377709	1.630299	-0.404015
6	1.283955	2.470370	-1.075196
6	-0.191730	2.080804	0.797592
6	1.627793	3.717317	-0.550180
1	1.719712	2.147509	-2.017995
6	0.144966	3.333089	1.318535
1	-0.899461	1.453241	1.330669
6	1.057302	4.152138	0.649247
1	2.331825	4.351579	-1.081588
1	-0.305709	3.666699	2.249315
1	1.316591	5.125626	1.055630
6	-1.602268	-0.487923	-0.402252
6	-1.707895	-1.202488	0.801879
6	-2.782813	-0.126036	-1.075340
6	-2.961008	-1.537956	1.321955
1	-0.810571	-1.497522	1.337276
6	-4.034716	-0.450499	-0.549908
1	-2.720725	0.410004	-2.019585
6	-4.126126	-1.160597	0.650421
1	-3.025065	-2.092372	2.254299
1	-4.936174	-0.159703	-1.082037
1	-5.098880	-1.422957	1.056643
6	1.223357	-1.143294	-0.402193
6	1.495588	-2.349848	-1.071690
6	1.901136	-0.873039	0.797072
6	2.404393	-3.270261	-0.546863
1	0.995222	-2.567866	-2.012429
6	2.820010	-1.789092	1.316568
1	1.710822	0.053742	1.329430
6	3.071195	-2.989966	0.649057
1	2.599316	-4.198768	-1.076193
1	3.337483	-1.563654	2.245069
1	3.786524	-3.699922	1.054462

Adduct Conc2

ΔE_{THF} -3775.59375799
ΔE_{THF}(ZPE) -3775.280258
ΔG_{THF} -3775.339631

6	-4.916577	-1.352897	0.001396
1	-4.583889	-1.857924	0.903944
1	-5.991635	-1.189212	-0.004713
1	-4.573313	-1.853686	-0.899507
15	0.675111	-0.003457	0.000944
46	-1.569446	0.124768	0.002381
35	-4.082742	0.454540	0.010719
6	1.443733	-0.514956	1.607160
6	0.825004	-0.088420	2.794892
6	2.604924	-1.298906	1.694378
6	1.362182	-0.423784	4.038348
1	-0.087150	0.501283	2.736876
6	3.135335	-1.644896	2.940585
1	3.096428	-1.644200	0.789701
6	2.518180	-1.206213	4.113813
1	0.872671	-0.083920	4.947070
1	4.032371	-2.256298	2.991724
1	2.931727	-1.476981	5.081447
6	1.397183	-1.200220	-1.214794
6	2.593145	-0.965743	-1.911166
6	0.704470	-2.401169	-1.445317
6	3.086041	-1.912864	-2.813811
1	3.141570	-0.041720	-1.753981
6	1.203776	-3.351589	-2.336440
1	-0.234898	-2.581306	-0.927168
6	2.395594	-3.107817	-3.025745
1	4.010571	-1.714404	-3.349451
1	0.657452	-4.276439	-2.501151
1	2.779814	-3.842549	-3.727992
6	1.536315	1.586868	-0.400183
6	0.964949	2.411650	-1.384844
6	2.717447	2.008029	0.230788
6	1.566611	3.618979	-1.739806
1	0.037788	2.105344	-1.863918
6	3.312959	3.224397	-0.117168
1	3.174382	1.391937	0.999290
6	2.741805	4.030422	-1.103694
1	1.112301	4.243507	-2.504328
1	4.224017	3.539049	0.384893
1	3.205140	4.975916	-1.371935

TS Conc2

ΔE_{THF} -3775.56797839
ΔE_{THF} (ZPE) -3775.256778
ΔG_{THF} -3775.314781

6	-3.562445	1.865874	0.079902
1	-4.058989	2.179168	-0.831440
1	-4.125789	2.077299	0.981410
1	-2.530843	2.317593	0.147992
15	0.625402	0.047999	0.003000
46	-1.586788	0.655566	0.027569
35	-4.002336	-0.289294	-0.044853
6	1.199547	-0.789667	1.548344
6	0.627057	-0.387394	2.767023
6	2.171483	-1.802443	1.558184
6	1.028799	-0.971763	3.969038
1	-0.143104	0.380843	2.766723
6	2.565116	-2.394538	2.761531
1	2.620153	-2.135028	0.626906
6	1.997873	-1.979013	3.968177
1	0.577832	-0.648562	4.903326
1	3.315419	-3.180588	2.753352
1	2.304253	-2.441726	4.902289
6	1.096385	-1.136512	-1.338741
6	2.322305	-1.079788	-2.019952
6	0.172534	-2.136484	-1.688376
6	2.617988	-2.005058	-3.025294
1	3.048063	-0.311573	-1.771115
6	0.473844	-3.066308	-2.684257
1	-0.788833	-2.178137	-1.182243
6	1.697215	-3.000768	-3.357422
1	3.569419	-1.945337	-3.546983
1	-0.250624	-3.834200	-2.941632
1	1.928304	-3.718184	-4.140010
6	1.823160	1.443063	-0.213107
6	1.461516	2.489224	-1.079456
6	3.060676	1.508510	0.445797
6	2.322025	3.566272	-1.294089
1	0.495927	2.459427	-1.579595
6	3.916480	2.594882	0.240218
1	3.358790	0.715033	1.124358
6	3.551449	3.623094	-0.630959
1	2.028390	4.365205	-1.969592
1	4.868898	2.634124	0.762030
1	4.217671	4.466796	-0.788468

Product Conc2

ΔE_{THF} -3775.60619919
ΔE_{THF}(ZPE) -3775.294397
ΔG_{THF} -3775.350285

6	3.158150	2.503491	0.050899
1	3.740565	2.422908	0.971891
1	3.806309	2.397741	-0.821844
1	2.591934	3.448959	0.016015
15	-0.523804	-0.025714	0.006254
46	1.602756	1.198889	0.026880
35	3.267337	-0.615929	0.033586
6	-0.828657	-1.204997	-1.370416
6	-0.082581	-1.051689	-2.550437
6	-1.775572	-2.238632	-1.288988
6	-0.290302	-1.906636	-3.634685
1	0.666215	-0.266492	-2.616319
6	-1.976951	-3.095764	-2.372744
1	-2.352814	-2.378107	-0.379830
6	-1.237162	-2.929777	-3.546701
1	0.294143	-1.779121	-4.541518
1	-2.710722	-3.893576	-2.298365
1	-1.394153	-3.599761	-4.387405
6	-1.001594	-0.931946	1.534929
6	-2.303343	-0.905976	2.060951
6	-0.010833	-1.682376	2.191970
6	-2.608914	-1.622187	3.220702
1	-3.077878	-0.323144	1.571425
6	-0.323369	-2.403410	3.345843
1	1.002921	-1.697793	1.800266
6	-1.621449	-2.373013	3.862890
1	-3.619073	-1.593130	3.619878
1	0.449434	-2.981733	3.844496
1	-1.861594	-2.929068	4.764849
6	-1.807081	1.285683	-0.180811
6	-1.794947	2.345667	0.746864
6	-2.721441	1.325260	-1.243860
6	-2.685192	3.411907	0.618198
1	-1.091979	2.333756	1.577523
6	-3.607295	2.399225	-1.373752
1	-2.744441	0.520963	-1.972267
6	-3.592308	3.442084	-0.445604
1	-2.667993	4.218894	1.345390
1	-4.310550	2.416568	-2.201748
1	-4.281810	4.274995	-0.549706

Adduct Conc1

ΔE_{THF} -3775.59384082

ΔE_{THF}(ZPE) -3775.280290
ΔG_{THF} -3775.339486

6	4.929984	1.330043	-0.047745
1	4.610553	1.864372	0.842724
1	6.003235	1.155179	-0.058288
1	4.583869	1.809014	-0.959431
15	-0.676341	-0.002630	0.001859
46	1.567820	-0.123790	0.007111
35	4.076901	-0.467354	0.019781
6	-1.362468	1.684779	-0.334094
6	-0.693896	2.787454	0.226370
6	-2.503259	1.914772	-1.118639
6	-1.163300	4.085054	0.020970
1	0.202941	2.621969	0.819405
6	-2.965348	3.216823	-1.334537
1	-3.033507	1.080034	-1.566744
6	-2.299859	4.303156	-0.763779
1	-0.636606	4.925881	0.464357
1	-3.847227	3.378468	-1.948730
1	-2.660259	5.314165	-0.932878
6	-1.515214	-1.068074	-1.259730
6	-2.744935	-1.707060	-1.036854
6	-0.878973	-1.239906	-2.501195
6	-3.325847	-2.495542	-2.034504
1	-3.251054	-1.595440	-0.082857
6	-1.465272	-2.017424	-3.500610
1	0.085062	-0.766835	-2.674223
6	-2.690151	-2.649899	-3.268032
1	-4.275751	-2.988252	-1.844790
1	-0.961068	-2.138336	-4.455634
1	-3.142314	-3.264437	-4.041690
6	-1.499483	-0.488043	1.588959
6	-0.917407	-1.525178	2.337777
6	-2.666705	0.122701	2.074233
6	-1.496240	-1.953033	3.533171
1	0.000057	-1.988107	1.981455
6	-3.239092	-0.298372	3.278354
1	-3.130572	0.930866	1.516393
6	-2.658319	-1.337936	4.007801
1	-1.034360	-2.757935	4.098612
1	-4.139887	0.187567	3.643766
1	-3.104554	-1.662866	4.943733

TS Conc1

ΔE_{THF} -3775.57018572
ΔE_{THF}(ZPE) -3775.258546
ΔG_{THF} -3775.317306

6	3.248609	1.677396	-0.298233
1	2.906596	2.068666	0.653246
1	4.249923	1.986178	-0.568044
1	2.541184	1.748835	-1.118691
15	-0.621360	-0.040468	0.009984
46	1.644003	-0.301879	0.059242
35	4.092338	-0.450381	0.093147
6	-1.175034	1.654912	-0.479639
6	-0.589420	2.751291	0.179750
6	-2.112937	1.899316	-1.493184
6	-0.944712	4.057399	-0.156856
1	0.147758	2.579239	0.960771
6	-2.458097	3.210290	-1.838882
1	-2.576787	1.069429	-2.016613
6	-1.878669	4.290350	-1.171788
1	-0.488056	4.892381	0.367581
1	-3.183739	3.382616	-2.629216
1	-2.149161	5.307547	-1.440968
6	-1.501125	-1.163364	-1.166536
6	-2.826562	-1.587312	-0.978273
6	-0.801191	-1.609679	-2.300127
6	-3.438081	-2.432485	-1.907593
1	-3.382613	-1.264366	-0.103139
6	-1.416375	-2.446846	-3.232765
1	0.233267	-1.304540	-2.441112
6	-2.736169	-2.861216	-3.036986
1	-4.462966	-2.755961	-1.747067
1	-0.861589	-2.782684	-4.104572
1	-3.213326	-3.520206	-3.757109
6	-1.485978	-0.332067	1.618055
6	-0.977110	-1.333820	2.462257
6	-2.621142	0.386013	2.025997
6	-1.598758	-1.623312	3.677636
1	-0.085014	-1.880641	2.165131
6	-3.236270	0.102426	3.248702
1	-3.024447	1.171411	1.393660
6	-2.729464	-0.903618	4.074246
1	-1.194274	-2.401963	4.318533
1	-4.112399	0.668524	3.553392
1	-3.208998	-1.121729	5.024497

Product Conc1

ΔE_{THF} -3775.63461253
ΔE_{THF}(ZPE) -3775.321205
ΔG_{THF} -3775.377321

6	-1.568869	1.381185	-1.738029
1	-2.148960	0.901982	-2.529811
1	-2.072976	2.278076	-1.369686
1	-0.558895	1.616137	-2.071935
46	-1.643333	0.095058	-0.166236
15	0.637163	0.002672	-0.017610
35	-4.152381	-0.014925	-0.067153
6	1.522308	1.609309	-0.073832
6	2.792672	1.755892	-0.651514
6	0.889650	2.731483	0.489302
6	3.421060	3.003873	-0.657898
1	3.292769	0.903476	-1.099723
6	1.524952	3.973467	0.488917
1	-0.103910	2.631803	0.918987
6	2.791259	4.111509	-0.086696
1	4.402428	3.107470	-1.111875
1	1.026651	4.833076	0.927688
1	3.281846	5.080615	-0.095338
6	1.465572	-1.105442	-1.224807
6	2.683249	-1.738274	-0.920359
6	0.872931	-1.324921	-2.478734
6	3.300099	-2.564687	-1.861009
1	3.145949	-1.594478	0.051688
6	1.495408	-2.149923	-3.417662
1	-0.080033	-0.861986	-2.715423
6	2.708918	-2.769321	-3.110761
1	4.239876	-3.050746	-1.615057
1	1.026899	-2.313709	-4.383821
1	3.189356	-3.415744	-3.839630
6	0.999997	-0.735831	1.626753
6	1.725714	-0.060890	2.619596
6	0.465840	-2.007833	1.909215
6	1.920224	-0.652486	3.870862
1	2.140924	0.921839	2.420828
6	0.664569	-2.593395	3.159218
1	-0.098739	-2.544000	1.150189
6	1.391499	-1.915803	4.142802
1	2.488302	-0.123464	4.630736
1	0.251109	-3.576554	3.364584
1	1.544322	-2.371624	5.116796

Adduct S_N21

ΔE_{THF} -3775.57624359
ΔE_{THF}(ZPE) -3775.263522
ΔG_{THF} -3775.323638

6	-3.698937	-0.022744	-0.239451
1	-3.368488	-0.321481	0.751397
1	-3.398447	-0.745111	-0.994193
1	-3.361940	0.979780	-0.488162
35	-5.681493	0.010620	-0.212563
15	1.008472	0.005160	-0.207499
46	-0.485500	0.053807	-1.826849
6	0.366359	-0.509023	1.453601
6	-0.528599	-1.592880	1.508712
6	0.719240	0.133925	2.649895
6	-1.048123	-2.027976	2.728278
1	-0.821400	-2.091844	0.587451
6	0.187547	-0.294708	3.870889
1	1.407941	0.972673	2.634126
6	-0.694921	-1.374857	3.913997
1	-1.734884	-2.869889	2.752176
1	0.467213	0.218360	4.787144
1	-1.108002	-1.705776	4.862819
6	1.840113	1.625643	0.134652
6	3.183115	1.733561	0.527748
6	1.084064	2.801342	-0.014365
6	3.754321	2.986891	0.767399
1	3.789777	0.840852	0.643865
6	1.650949	4.051105	0.237455
1	0.048955	2.729088	-0.340814
6	2.990473	4.147085	0.625827
1	4.797419	3.053146	1.065047
1	1.051329	4.949623	0.118692
1	3.436883	5.120319	0.810612
6	2.430783	-1.150282	-0.484078
6	2.906233	-1.308771	-1.797291
6	3.050319	-1.869043	0.549951
6	3.985194	-2.150974	-2.067312
1	2.416052	-0.774305	-2.608190
6	4.123750	-2.722699	0.276635
1	2.693950	-1.769567	1.570985
6	4.595305	-2.862924	-1.029901
1	4.341530	-2.261310	-3.087987
1	4.589157	-3.276649	1.087543
1	5.428040	-3.528184	-1.241098

TS S_N21

ΔE_{THF} -3775.56738612
ΔE_{THF}(ZPE) -3775.255353
ΔG_{THF} -3775.313777

6	2.801657	-0.127439	-0.722797
1	2.560417	0.793881	-0.217168
1	2.982653	-0.105292	-1.792926
1	2.599595	-1.064821	-0.226906
35	5.055261	-0.087585	-0.222439
15	-0.865855	-0.002408	-0.131724
46	0.641906	-0.335711	-1.757940
6	-0.564832	-0.958892	1.420498
6	0.535111	-0.617401	2.228799
6	-1.343823	-2.070887	1.774382
6	0.840736	-1.365195	3.365663
1	1.151688	0.241146	1.976541
6	-1.030871	-2.822759	2.911330
1	-2.195707	-2.355520	1.165040
6	0.059408	-2.473209	3.709117
1	1.690424	-1.083411	3.981269
1	-1.646194	-3.679519	3.172187
1	0.300165	-3.057773	4.592511
6	-2.574123	-0.488368	-0.646006
6	-3.727173	0.142865	-0.152450
6	-2.716948	-1.535033	-1.572928
6	-4.993388	-0.268950	-0.574676
1	-3.641180	0.961191	0.555515
6	-3.983900	-1.952957	-1.984642
1	-1.828747	-2.018328	-1.974028
6	-5.124821	-1.318116	-1.487885
1	-5.876924	0.232514	-0.189290
1	-4.077877	-2.766344	-2.698791
1	-6.111158	-1.635087	-1.814993
6	-1.035581	1.742655	0.445531
6	-0.732481	2.774067	-0.458602
6	-1.476887	2.078789	1.736287
6	-0.878586	4.111518	-0.086203
1	-0.373393	2.521780	-1.453800
6	-1.615438	3.417777	2.109493
1	-1.705686	1.297709	2.455104
6	-1.318693	4.435538	1.199598
1	-0.639437	4.898341	-0.796237
1	-1.954650	3.663658	3.111994
1	-1.424176	5.476143	1.493404

Product S_N21

ΔE_{THF} -3775.59103813
ΔE_{THF}(ZPE) -3775.277845
ΔG_{THF} -3775.334083

6	-2.010553	0.075606	-0.884836
1	-2.062551	-0.512588	0.030296
1	-2.682084	-0.334882	-1.648774
1	-2.208725	1.133681	-0.697016
35	-5.683129	0.017036	-0.381798
15	0.959139	0.022132	-0.006592
46	-0.271578	-0.066935	-1.885331
6	0.836321	1.541852	1.008972
6	-0.333830	1.760229	1.759401
6	1.863110	2.499290	1.040359
6	-0.468566	2.914847	2.528354
1	-1.135985	1.028902	1.758587
6	1.718749	3.655479	1.812030
1	2.776962	2.348656	0.476007
6	0.555950	3.865946	2.554466
1	-1.374397	3.069680	3.106742
1	2.521918	4.386193	1.834476
1	0.447920	4.764616	3.154635
6	2.673395	-0.093043	-0.649311
6	3.576155	-1.052968	-0.164866
6	3.074427	0.766059	-1.691262
6	4.858999	-1.145286	-0.708867
1	3.282820	-1.726342	0.633651
6	4.358718	0.670041	-2.227332
1	2.388040	1.513238	-2.086792
6	5.251968	-0.286869	-1.738041
1	5.549881	-1.890739	-0.326306
1	4.657798	1.340028	-3.027872
1	6.249548	-0.364877	-2.160053
6	0.717325	-1.377247	1.141609
6	0.109071	-2.552978	0.675177
6	1.171373	-1.309942	2.470045
6	-0.040247	-3.650402	1.524047
1	-0.257169	-2.600679	-0.346599
6	1.019645	-2.411059	3.313654
1	1.635331	-0.403819	2.847338
6	0.414834	-3.579788	2.842479
1	-0.519876	-4.553189	1.157959
1	1.370867	-2.353609	4.339614
1	0.293665	-4.432094	3.504659

Adduct S_N22

ΔE_{THF} -3775.57828606
ΔE_{THF}(ZPE) -3775.265652
ΔG_{THF} -3775.323522

6	3.746820	-1.117516	-0.052520
1	3.183008	-0.968888	0.884805
1	3.194265	-0.900449	-0.982437
1	4.137460	-2.130641	-0.086739
35	5.281598	0.121897	0.002398
46	1.348850	-0.451324	-0.029100
15	-0.856482	-0.033518	-0.002043
6	-1.747442	-0.635242	1.503947
6	-1.308465	-1.832436	2.094603
6	-2.834540	0.043735	2.076890
6	-1.951273	-2.348070	3.220609
1	-0.452598	-2.352434	1.670312
6	-3.470032	-0.467790	3.212115
1	-3.185476	0.974918	1.642186
6	-3.032800	-1.664565	3.783635
1	-1.601120	-3.276108	3.664345
1	-4.307203	0.071076	3.647620
1	-3.527512	-2.059462	4.666721
6	-1.293116	1.762777	-0.078726
6	-2.390650	2.259841	-0.798406
6	-0.474719	2.667443	0.619919
6	-2.664058	3.630981	-0.815295
1	-3.032627	1.580940	-1.351378
6	-0.755993	4.033892	0.612089
1	0.390629	2.294115	1.163074
6	-1.850843	4.519426	-0.109127
1	-3.514639	4.001635	-1.381030
1	-0.114362	4.719679	1.158621
1	-2.064381	5.584625	-0.125047
6	-1.807905	-0.779242	-1.402798
6	-1.195397	-0.822587	-2.667268
6	-3.102589	-1.301969	-1.259995
6	-1.867219	-1.360741	-3.765299
1	-0.183985	-0.439867	-2.783398
6	-3.769827	-1.852106	-2.358525
1	-3.592742	-1.285467	-0.291465
6	-3.156254	-1.880045	-3.612288
1	-1.380664	-1.384575	-4.736601
1	-4.769936	-2.257629	-2.231111
1	-3.676102	-2.308913	-4.464542

TS S_N22

ΔE_{THF} -3775.55510814
ΔE_{THF}(ZPE) -3775.245259
ΔG_{THF} -3775.301365

6	-3.448380	0.006371	0.011768
1	-3.541072	1.045433	-0.299884
1	-3.540622	-0.242750	1.067627
1	-3.545051	-0.783250	-0.731262
35	-5.998381	0.008369	0.012661
46	-1.356989	0.011159	0.013517
15	1.035588	0.003524	0.003863
6	1.800946	1.527122	-0.705812
6	1.132281	2.160918	-1.767557
6	3.000604	2.081425	-0.233070
6	1.660582	3.310078	-2.356682
1	0.191341	1.752504	-2.130473
6	3.522832	3.238933	-0.816907
1	3.527534	1.615830	0.594444
6	2.857132	3.852899	-1.880094
1	1.133406	3.786432	-3.178573
1	4.450702	3.658933	-0.438601
1	3.264661	4.753168	-2.331267
6	1.812630	-0.159319	1.670277
6	2.990691	-0.885753	1.903408
6	1.180858	0.476360	2.753048
6	3.526351	-0.969713	3.191547
1	3.488980	-1.391838	1.081994
6	1.723213	0.401302	4.036398
1	0.258326	1.029061	2.588657
6	2.897152	-0.324486	4.258196
1	4.436399	-1.539301	3.358601
1	1.224883	0.899923	4.863001
1	3.315439	-0.391462	5.258557
6	1.772491	-1.377043	-0.976146
6	1.111629	-2.617568	-0.953089
6	2.941130	-1.244991	-1.742059
6	1.615568	-3.705376	-1.666551
1	0.196844	-2.727240	-0.374129
6	3.438904	-2.332712	-2.464804
1	3.462648	-0.293434	-1.778511
6	2.780194	-3.563448	-2.426621
1	1.095150	-4.658546	-1.636722
1	4.342392	-2.215839	-3.056866
1	3.168221	-4.406688	-2.990984

Product S_N22

ΔE_{THF} -3775.55659258
ΔE_{THF}(ZPE) -3775.245863
ΔG_{THF} -3775.302130

6	-3.355087	-0.063859	-0.074237
1	-3.603277	0.940635	-0.425400
1	-3.597232	-0.260043	0.973231
1	-3.618189	-0.868569	-0.764191
35	-6.302161	0.008201	0.003082
46	-1.333392	-0.046868	-0.066133
15	1.128911	0.001541	-0.005162
6	1.860523	1.615548	-0.514335
6	1.201008	2.350482	-1.515374
6	3.031853	2.138942	0.054033
6	1.713596	3.572890	-1.951228
1	0.281522	1.967165	-1.953503
6	3.538207	3.367706	-0.377814
1	3.548750	1.591612	0.836265
6	2.883384	4.084004	-1.381721
1	1.195626	4.129142	-2.727276
1	4.444657	3.763395	0.071837
1	3.278581	5.039582	-1.714639
6	1.831640	-0.331493	1.665266
6	2.987908	-1.098613	1.873523
6	1.157764	0.203201	2.777059
6	3.462665	-1.320666	3.169046
1	3.516234	-1.527600	1.027513
6	1.639372	-0.011385	4.068858
1	0.254204	0.791517	2.630575
6	2.792484	-0.776303	4.266635
1	4.356783	-1.919672	3.317790
1	1.110333	0.410009	4.919011
1	3.162957	-0.951294	5.272720
6	1.918509	-1.244012	-1.106982
6	1.266238	-2.478411	-1.268396
6	3.125409	-1.015699	-1.785807
6	1.815209	-3.469441	-2.083225
1	0.325191	-2.661142	-0.752542
6	3.668553	-2.006067	-2.607989
1	3.638957	-0.065162	-1.678109
6	3.017164	-3.232930	-2.756194
1	1.301632	-4.419701	-2.198651
1	4.601497	-1.817421	-3.131809
1	3.441394	-4.000055	-3.397875

2.2.3 Species Optimized in DMF

2.2.3.1 PF_3

$PdPF_3$

ΔE_{DMF} -768.952989274
ΔE_{DMF}(ZPE) -768.944004
ΔG_{DMF} -768.974560

46	0.000000	0.000000	1.262317
15	0.000000	0.000000	-0.826240
9	0.000000	1.381017	-1.691592
9	-1.195996	-0.690509	-1.691592
9	1.195996	-0.690509	-1.691592

PF_3

ΔE_{DMF} -640.986852414
ΔE_{DMF}(ZPE) -640.979035
ΔG_{DMF} -641.005300

15	0.000000	0.000000	0.526146
9	0.000000	1.393676	-0.292303
9	1.206959	-0.696838	-0.292303
9	-1.206959	-0.696838	-0.292303

Adduct Conc2

ΔE_{DMF} -3380.29566305
ΔE_{DMF}(ZPE) -3380.248467
ΔG_{DMF} -3380.290460

15	-2.187720	0.041244	0.001272
46	-0.069768	-0.009368	-0.006523
35	2.509814	-0.434996	0.003453
6	3.317099	1.384286	0.002126
1	2.956328	1.888039	0.894099
1	4.392461	1.227899	0.023869
1	2.990331	1.871640	-0.911807
9	-3.069350	-0.911982	-0.972564
9	-3.044895	-0.294245	1.338793
9	-3.003540	1.399983	-0.350541

TS Conc2

ΔE_{DMF} -3380.26251059
ΔE_{DMF}(ZPE) -3380.217399
ΔG_{DMF} -3380.254834

15	2.003375	-0.140619	-0.000005
46	-0.098100	0.495220	0.000106
35	-2.350237	-0.717977	-0.000043
6	-2.056171	1.561733	-0.000195
1	-2.615999	1.731753	-0.911739
1	-2.616152	1.731925	0.911225
1	-1.100211	2.160759	-0.000176
9	2.584004	-1.037169	1.207685
9	2.576949	-1.059740	-1.194003
9	3.215674	0.926193	-0.013845

Product Conc2

ΔE_{DMF} -3380.29057650
ΔE_{DMF}(ZPE) -3380.244744
ΔG_{DMF} -3380.286240

15	-1.770041	0.026170	-0.000044
46	0.425125	-0.901815	-0.000147
35	1.499719	1.325409	-0.000004
6	2.294251	-1.668775	0.000301
1	2.837856	-1.386279	-0.901835
1	2.837744	-1.385925	0.902387
1	2.012403	-2.732791	0.000501
9	-3.099785	-0.868072	-0.000041
9	-2.169722	1.002072	-1.202048
9	-2.169250	1.001474	1.202609

Adduct Conc1

ΔE_{DMF} -3380.29566290
ΔE_{DMF}(ZPE) -3380.248467
ΔG_{DMF} -3380.290460

15	-2.187805	0.041102	0.001274
46	-0.069847	-0.009014	-0.006551
35	2.509793	-0.435128	0.003489
6	3.317917	1.383759	0.002063
1	2.957125	1.887901	0.893810
1	4.393205	1.226913	0.024152
1	2.991665	1.871108	-0.912063
9	-3.069414	-0.912078	-0.972670
9	-3.044923	-0.294517	1.338765
9	-3.003688	1.399832	-0.350339

TS Conc1

ΔE_{DMF} -3380.26428025
ΔE_{DMF}(ZPE) -3380.218737
ΔG_{DMF} -3380.256850

6	-1.457357	1.890344	-0.001152
1	-0.904579	2.072308	-0.917360
1	-2.471923	2.261324	-0.020526
1	-0.936576	2.075702	0.932773
15	2.043247	-0.018080	-0.000308
46	-0.118118	-0.218347	-0.002663
35	-2.560288	-0.258285	0.001979
9	2.743176	1.385686	-0.375312
9	2.964326	-0.930527	-0.960700
9	2.898280	-0.276965	1.343774

Product Conc1

ΔE_{DMF} -3380.30907788
ΔE_{DMF}(ZPE) -3380.262100
ΔG_{DMF} -3380.301817

46	0.218632	-0.097553	-0.000001
15	-2.009324	-0.145584	-0.000078
6	0.163410	1.951988	-0.000893
1	-0.381846	2.269458	0.889448
1	1.202863	2.269877	0.028660
1	-0.329532	2.260380	-0.924342
35	2.678221	-0.198432	0.000491
9	-2.824767	0.624559	-1.129338
9	-2.817712	0.401311	1.257953
9	-2.704955	-1.569798	-0.129104

Adduct S_N21

ΔE_{DMF} -3380.28331802
ΔE_{DMF}(ZPE) -3380.236264
ΔG_{DMF} -3380.280950

6	-2.387310	0.284991	0.104657
1	-2.015095	0.754886	-0.801838
1	-2.130933	0.860320	0.990300
1	-2.057508	-0.748127	0.186647
35	-4.362813	0.255173	-0.020326
15	2.566359	0.441353	-0.004468
46	1.054327	-1.002099	-0.001342
9	4.011035	0.171515	-0.707374
9	3.204028	1.028498	1.374988
9	2.366206	1.907559	-0.685714

TS S_N21

ΔE_{DMF} -3380.26185463
ΔE_{DMF}(ZPE) -3380.215760
ΔG_{DMF} -3380.256043

6	-1.173877	-0.180088	-0.005660
1	-1.037228	0.558729	-0.779294
1	-1.133979	0.124491	1.030057
1	-1.488960	-1.184851	-0.271757
35	-3.614874	0.374173	0.000813
15	2.036980	0.595442	-0.000017
46	0.856729	-1.193414	0.000968
9	3.135732	0.847287	-1.148217
9	3.001506	0.941614	1.241045
9	1.336075	2.039045	-0.094802

Product S_N21

ΔE_{DMF} -3380.26733982
ΔE_{DMF}(ZPE) -3380.220887
ΔG_{DMF} -3380.263362

6	-0.760075	-0.268992	-0.013134
1	-0.838011	0.476143	-0.801076
1	-0.938038	0.134544	0.981947
1	-1.328244	-1.180199	-0.227919
35	-3.953871	0.318290	0.001451
15	2.082238	0.693833	0.000331
46	1.048694	-1.217616	0.002695
9	3.654176	0.655515	-0.216049
9	2.036502	1.620679	1.289219
9	1.706734	1.795601	-1.079157

Adduct S_N22

ΔE_{DMF} -3380.28322252
ΔE_{DMF}(ZPE) -3380.235991
ΔG_{DMF} -3380.280004

6	-2.779968	0.738258	0.144280
1	-2.185198	0.209464	0.885831
1	-2.326033	0.692177	-0.842801
1	-2.978384	1.763253	0.446912
35	-4.524070	-0.185828	0.029227
46	0.820122	0.073997	-0.151893
15	2.895436	-0.059277	0.054668
9	3.594000	-0.630111	1.411387
9	3.806903	-0.964864	-0.946779
9	3.860730	1.249957	-0.043665

2.2.3.2 PH_3

$PdPH_3$

ΔE_{DMF} -471.095897500
ΔE_{DMF} (ZPE) -471.069098
ΔG_{DMF} -471.095920

46	-0.645402	-0.000003	0.000001
15	1.527889	-0.000008	0.000005
1	2.256457	1.203891	-0.186827
1	2.256912	-0.440048	1.135806
1	2.256802	-0.763596	-0.949099

PH_3

ΔE_{DMF} -343.146002145
ΔE_{DMF} (ZPE) -343.121982
ΔG_{DMF} -343.143023

15	-0.000002	-0.000007	-0.126104
1	0.159683	1.192757	0.630506
1	-1.112793	-0.458055	0.630525
1	0.953146	-0.734602	0.630530

Adduct Conc2

ΔE_{DMF} -3082.44297320
ΔE_{DMF} (ZPE) -3082.378078
ΔG_{DMF} -3082.414635

15	-2.924177	0.166500	0.000204
46	-0.714655	-0.033656	0.000091
35	1.802875	-0.422714	-0.000217
1	-3.517707	1.453400	0.000496
1	-3.701883	-0.368494	-1.056868
1	-3.701798	-0.368931	1.057117
6	2.682765	1.367091	-0.000054
1	3.286090	1.410924	0.902810
1	3.287532	1.410361	-0.901981
1	1.887362	2.105851	-0.000920

TS Conc2

ΔE_{DMF} -3082.41669305
ΔE_{DMF}(ZPE) -3082.353931
ΔG_{DMF} -3082.390466

15	-2.743090	-0.403825	0.000038
46	-0.563191	0.252782	0.000002
35	1.871635	-0.547580	-0.000018
1	-3.786528	0.553563	-0.000008
1	-3.245059	-1.196260	-1.059299
1	-3.245052	-1.196149	1.059462
6	1.314344	1.609399	-0.000020
1	1.835163	1.882216	0.910065
1	1.835165	1.882210	-0.910105
1	0.266175	2.012715	-0.000024

Product Conc2

ΔE_{DMF} -3082.45627075
ΔE_{DMF}(ZPE) -3082.393027
ΔG_{DMF} -3082.429585

15	2.286672	-0.877854	-0.000017
46	0.380703	0.688189	0.000006
35	-1.437513	-0.983216	0.000000
1	3.616810	-0.399475	-0.000173
1	2.409258	-1.796668	1.065223
1	2.409123	-1.797126	-1.064878
6	-1.040631	2.123136	-0.000010
1	-1.659320	2.089023	-0.899361
1	-1.658889	2.089561	0.899658
1	-0.372646	2.999571	-0.000447

Adduct Conc1

ΔE_{DMF} -3082.44344309
ΔE_{DMF}(ZPE) -3082.378418
ΔG_{DMF} -3082.416318

15	-2.921577	0.163665	0.000016
46	-0.710709	-0.033408	-0.000016
35	1.802575	-0.423458	0.000009
1	-3.518234	1.449112	-0.000255
1	-3.698171	-0.373551	-1.056742
1	-3.697979	-0.373044	1.057170
6	2.659086	1.374422	0.000004
1	3.731209	1.193799	0.000183
1	2.327535	1.879931	-0.902470
1	2.327259	1.880068	0.902299

TS Conc1

ΔE_{DMF} -3082.41773972
ΔE_{DMF}(ZPE) -3082.354557
ΔG_{DMF} -3082.391712

6	-1.127752	1.842697	-0.000010
1	-0.068406	2.094951	0.000005
1	-1.641057	2.102719	-0.916285
1	-1.641057	2.102644	0.916287
15	2.797493	-0.016334	-0.000037
46	0.530140	-0.110994	0.000038
35	-1.907393	-0.343397	-0.000023
1	3.491280	0.612666	1.061005
1	3.490939	0.618858	-1.057613
1	3.544739	-1.218376	-0.003721

Product Conc1

ΔE_{DMF} -3082.47908728
ΔE_{DMF}(ZPE) -3082.414528
ΔG_{DMF} -3082.451207

46	-0.393660	-0.150506	-0.000095
15	-2.675932	-0.346612	0.000099
1	-3.401439	0.214270	-1.068852
1	-3.178155	-1.663514	-0.017662
1	-3.397335	0.183418	1.087456
6	-0.630552	1.867007	0.000026
1	-1.180782	2.155143	0.898813
1	0.377990	2.278775	0.006284
1	-1.169688	2.154838	-0.905569
35	2.113715	-0.125786	0.000064

Adduct S_N21

ΔE_{DMF} -3082.42682180
ΔE_{DMF}(ZPE) -3082.362243
ΔG_{DMF} -3082.403393

6	-1.644816	0.250949	0.051562
1	-1.324468	0.685072	-0.891597
1	-1.394937	0.888724	0.894991
1	-1.260125	-0.757506	0.181490
35	-3.623444	0.114281	-0.009647
15	3.097069	1.140068	-0.005244
1	4.108440	1.296853	-0.988304
1	2.549280	2.441943	-0.142823
1	3.921576	1.440063	1.110078
46	1.818123	-0.621776	-0.001237

TS S_N21

ΔE_{DMF} -3082.41791735
ΔE_{DMF}(ZPE) -3082.354568
ΔG_{DMF} -3082.392815

6	-0.798069	0.056917	-0.005512
1	-0.736477	-0.418321	0.965307
1	-0.749580	-0.532749	-0.912966
1	-0.650750	1.122438	-0.071008
35	-3.124670	0.163414	0.000800
46	1.497742	-0.670444	0.000400
15	2.575350	1.264651	0.000253
1	3.472515	1.569669	1.051705
1	3.439620	1.589227	-1.072675
1	1.850172	2.479380	0.022526

Product S_N21

ΔE_{DMF} -3082.44421017
ΔE_{DMF}(ZPE) -3082.379941
ΔG_{DMF} -3082.419411

6	0.179143	-0.197317	-0.000036
1	-0.108389	0.412111	-0.858035
1	-0.112283	0.270770	0.941968
1	-0.215325	-1.218456	-0.084454
35	-4.172691	0.079628	0.000025
15	2.597045	1.524803	-0.000134
1	3.973983	1.813713	0.004544
1	2.143583	2.288288	-1.089672
1	2.135540	2.288878	1.085583
46	2.134707	-0.659357	0.000030

Adduct S_N22

ΔE_{DMF} -3082.42689673
ΔE_{DMF}(ZPE) -3082.362873
ΔG_{DMF} -3082.399908

35	-2.876565	-0.260698	0.000004
46	1.104184	0.149850	-0.000059
15	3.263271	-0.344170	0.000084
1	3.676886	-1.698644	-0.011287
1	4.101109	0.096044	-1.053265
1	4.096754	0.076853	1.064681
6	-1.298467	0.921748	0.000110
1	-1.649874	1.949741	0.000987
1	-0.747507	0.719078	0.933001
1	-0.748326	0.720306	-0.933484

TS S_N22

ΔE_{DMF} -3082.40617184
ΔE_{DMF}(ZPE) -3082.344498
ΔG_{DMF} -3082.382439

6	-0.871035	-0.030672	-0.000234
1	-0.913928	-0.570760	0.942690
1	-0.914071	-0.578986	-0.938394
1	-0.897868	1.056773	-0.005014
35	-3.339130	0.011208	0.000019
46	1.254542	-0.013132	0.000046
15	3.609205	0.025072	-0.000030
1	4.335976	-0.597390	-1.042737
1	4.303421	1.257931	-0.028648
1	4.335216	-0.547861	1.071190

Product S_N22

ΔE_{DMF} -3082.41302524
ΔE_{DMF}(ZPE) -3082.350918
ΔG_{DMF} -3082.387611

35	3.892734	-0.025450	0.000055
46	-1.477455	0.036903	-0.000599
15	-3.988614	-0.070917	0.000406
1	-4.627124	-1.116466	-0.700270
1	-4.669820	-0.209802	1.228753
1	-4.738597	1.005180	-0.521430
6	0.524274	0.063618	0.001114
1	0.818988	-0.823250	-0.567606
1	0.808258	1.002471	-0.483003
1	0.809091	0.017120	1.056409

2.2.3.3 $P(CH_3)_3$

$PdP(CH_3)_3$

ΔE_{DMF} -589.073012436
ΔE_{DMF} (ZPE) -588.958979
ΔG_{DMF} -588.992602

46	-1.324849	-0.000145	0.000047
15	0.873042	0.000079	-0.000086
6	1.718050	-1.035500	-1.287417
1	1.417338	-0.699865	-2.283919
1	2.808330	-0.961522	-1.196608
1	1.418451	-2.080903	-1.171427
6	1.718189	-0.597187	1.540316
1	1.420830	-1.629610	1.744649
1	2.808492	-0.551501	1.432335
1	1.415489	0.022611	2.389010
6	1.716866	1.633353	-0.252999
1	1.415144	2.328169	0.535801
1	2.807234	1.518680	-0.233680
1	1.417465	2.055439	-1.216445

$P(CH_3)_3$

ΔE_{DMF} -461.116066898
ΔE_{DMF}(ZPE) -461.003674
ΔG_{DMF} -461.033062

15	0.000324	-0.000595	-0.593850
6	1.524521	-0.626793	0.275249
1	1.715810	-1.662928	-0.021992
1	2.388991	-0.025481	-0.024084
1	1.423362	-0.583670	1.366419
6	-0.219052	1.633258	0.274544
1	0.580897	2.317927	-0.025160
1	-1.173515	2.080116	-0.021736
1	-0.202248	1.524636	1.365763
6	-1.305851	-1.005730	0.274988
1	-2.298052	-0.653081	-0.024565
1	-1.217831	-2.055820	-0.021749
1	-1.219986	-0.937181	1.366165

Adduct Conc2

ΔE_{DMF} -3200.42112693
ΔE_{DMF}(ZPE) -3200.268884
ΔG_{DMF} -3200.312658

15	2.247668	0.059168	-0.000013
46	0.002265	-0.063557	-0.000083
35	-2.507330	-0.409183	-0.000003
6	-3.369274	1.387717	0.000083
1	-4.441148	1.205343	-0.000107
1	-3.038887	1.894446	0.902405
1	-3.038594	1.894679	-0.901999
6	2.982089	1.761357	-0.002236
1	4.077432	1.717937	-0.001945
1	2.645077	2.304511	-0.889699
1	2.644724	2.307037	0.883543
6	3.132128	-0.714888	1.433609
1	4.217652	-0.598703	1.335288
1	2.803252	-0.243518	2.364081
1	2.888504	-1.779937	1.482906
6	3.132900	-0.718838	-1.431023
1	2.804723	-0.249833	-2.362939
1	4.218372	-0.602542	-1.332277
1	2.889168	-1.783981	-1.477717

TS Conc2

ΔE_{DMF} -3200.39525202
ΔE_{DMF}(ZPE) -3200.245026
ΔG_{DMF} -3200.286643

15	-2.116848	-0.124378	-0.000231
46	0.119114	0.385952	0.000641
35	2.498097	-0.626428	-0.000490
6	2.130792	1.549706	-0.001382
1	2.670419	1.792092	0.906814
1	2.667966	1.791168	-0.911262
1	1.111759	2.030369	-0.000054
6	-3.309380	1.284225	-0.170428
1	-4.345178	0.926298	-0.161530
1	-3.165094	1.986973	0.655080
1	-3.120379	1.812497	-1.109259
6	-2.701909	-1.260104	-1.341441
1	-3.778990	-1.444450	-1.258058
1	-2.488975	-0.814794	-2.317405
1	-2.167703	-2.211968	-1.273355
6	-2.765761	-0.973173	1.512263
1	-2.600245	-0.339696	2.388250
1	-3.837329	-1.181462	1.416574
1	-2.228655	-1.914113	1.661257

Product Conc2

ΔE_{DMF} -3200.43708593
ΔE_{DMF}(ZPE) -3200.286740
ΔG_{DMF} -3200.328992

15	1.834517	-0.105528	-0.000081
46	-0.409399	0.865901	-0.000233
35	-1.680736	-1.252414	0.000005
6	-2.188921	1.855289	0.000305
1	-2.782511	1.649785	-0.894246
1	-2.775586	1.656907	0.901090
1	-1.806663	2.889507	-0.005354
6	2.244067	-1.181795	1.443214
1	3.260340	-1.581539	1.362200
1	2.158664	-0.602382	2.367034
1	1.532718	-2.010966	1.488826
6	2.244697	-1.183560	-1.441854
1	2.159920	-0.605256	-2.366425
1	3.260854	-1.583383	-1.359758
1	1.533235	-2.012665	-1.486862
6	3.219395	1.119786	-0.000498
1	4.192283	0.616952	0.000036
1	3.146070	1.754836	-0.888055
1	3.145636	1.755868	0.886280

Adduct Conc1

ΔE_{DMF} -3200.42112695
ΔE_{DMF}(ZPE) -3200.268883
ΔG_{DMF} -3200.312656

15	-2.247677	0.059181	0.000030
46	-0.002264	-0.063442	0.000083
35	2.507328	-0.409222	-0.000034
6	3.369221	1.387693	0.000007
1	3.039768	1.894002	0.902906
1	4.441105	1.205386	-0.001386
1	3.037597	1.895081	-0.901486
6	-2.982373	1.761242	-0.005456
1	-4.077711	1.717689	-0.004958
1	-2.644992	2.308759	0.879187
1	-2.645531	2.302670	-0.894038
6	-3.132411	-0.721649	-1.429756
1	-4.217958	-0.605702	-1.331415
1	-2.804288	-0.254059	-2.362398
1	-2.888162	-1.786753	-1.474613
6	-3.132280	-0.712382	1.434899
1	-2.803777	-0.239148	2.364558
1	-4.217804	-0.596677	1.336058
1	-2.888380	-1.777265	1.486324

TS Conc1

ΔE_{DMF} -3200.39695539
ΔE_{DMF}(ZPE) -3200.246525
ΔG_{DMF} -3200.288696

6	1.735114	1.854564	0.001791
1	1.289150	2.065521	0.967759
1	2.751044	2.211659	-0.100754
1	1.112633	2.063543	-0.862412
15	-2.131235	-0.007089	0.000818
46	0.146393	-0.172375	-0.000823
35	2.597116	-0.308770	0.000781
6	-3.046190	-1.333343	-0.912466
1	-2.738157	-1.335023	-1.961850
1	-2.803263	-2.308450	-0.480794
1	-4.129054	-1.175124	-0.855577
6	-2.967015	-0.051339	1.652755
1	-4.054339	0.033655	1.545977
1	-2.728331	-0.991766	2.157502
1	-2.601801	0.773492	2.271171
6	-2.853593	1.526983	-0.742062
1	-2.544974	1.606747	-1.788264
1	-3.948048	1.513853	-0.689736
1	-2.479374	2.403243	-0.204878

Product Conc1

ΔE_{DMF} -3200.46664727
ΔE_{DMF}(ZPE) -3200.314761
ΔG_{DMF} -3200.356241

46	0.230219	-0.033174	-0.001226
15	-2.053190	-0.155896	-0.000480
6	0.097923	1.991319	0.001391
1	-0.554079	2.337897	0.806527
1	1.119018	2.343562	0.154371
1	-0.282483	2.309876	-0.972596
35	2.752921	-0.220508	0.000961
6	-2.960396	0.817268	-1.268929
1	-4.034095	0.615490	-1.203339
1	-2.787983	1.884964	-1.112316
1	-2.600799	0.545643	-2.264650
6	-2.883087	0.283811	1.581472
1	-2.701709	1.335862	1.816423
1	-3.962011	0.114011	1.505961
1	-2.475498	-0.330209	2.388569
6	-2.565847	-1.896938	-0.309499
1	-2.137190	-2.548222	0.456721
1	-3.657064	-1.980564	-0.283631
1	-2.202147	-2.218827	-1.288669

Adduct S_N21

ΔE_{DMF} -3200.40445943
ΔE_{DMF}(ZPE) -3200.252389
ΔG_{DMF} -3200.296380

6	2.372426	0.514253	0.008414
1	1.973907	0.043784	0.904013
1	2.224151	1.590908	0.020022
1	1.967503	0.062415	-0.893907
35	4.330601	0.196719	-0.001804
15	-2.672343	0.368261	-0.000603
46	-0.863169	-0.886200	0.000441
6	-2.443248	2.201534	-0.165188
1	-1.928349	2.424274	-1.103881
1	-3.409958	2.719069	-0.153642
1	-1.829063	2.570878	0.660815
6	-3.752658	0.281059	1.505005
1	-3.181483	0.588720	2.385350
1	-4.627105	0.933777	1.396878
1	-4.089719	-0.748344	1.655727
6	-3.911320	0.044874	-1.342913
1	-4.772632	0.717030	-1.250022
1	-3.442596	0.194487	-2.319538
1	-4.255993	-0.991202	-1.281800

TS S_N21

ΔE_{DMF} -3200.39726697
ΔE_{DMF}(ZPE) -3200.246445
ΔG_{DMF} -3200.290067

6	1.474731	-0.128722	-0.019825
1	1.252906	0.156007	0.997732
1	1.182274	0.540802	-0.813149
1	1.609443	-1.178126	-0.254108
35	3.688061	0.381585	0.002799
15	-2.159262	0.572572	-0.001706
46	-0.790231	-1.186197	0.000304
6	-1.422764	2.232444	-0.355728
1	-0.965969	2.230073	-1.349297
1	-2.192119	3.011791	-0.317268
1	-0.648086	2.458555	0.382179
6	-3.059230	0.893429	1.584422
1	-2.337953	1.075282	2.385741
1	-3.717468	1.764463	1.487319
1	-3.657913	0.017776	1.849752
6	-3.553961	0.512886	-1.218337
1	-4.186687	1.403061	-1.125632
1	-3.153206	0.460067	-2.234262
1	-4.160467	-0.378964	-1.038527

Product S_N21

ΔE_{DMF} -3200.43593013
ΔE_{DMF}(ZPE) -3200.284115
ΔG_{DMF} -3200.328344

6	0.423918	-0.234098	0.224565
1	0.434744	0.447309	1.077253
1	0.702871	0.282604	-0.696176
1	1.081565	-1.094037	0.409411
35	4.834797	0.249364	-0.021040
15	-2.417744	0.745832	-0.010420
46	-1.316536	-1.206683	-0.018791
6	-1.729188	2.096466	-1.039972
1	-1.619562	1.752906	-2.071126
1	-2.403668	2.957796	-1.011456
1	-0.750244	2.394965	-0.658504
6	-2.649116	1.480032	1.654835
1	-1.677787	1.736311	2.084204
1	-3.261115	2.384513	1.580047
1	-3.145295	0.757587	2.307169
6	-4.111793	0.454800	-0.656769
1	-4.685121	1.386931	-0.620861
1	-4.055725	0.103468	-1.689791
1	-4.614687	-0.301365	-0.049047

Adduct S_N22

ΔE_{DMF} -3200.40538917
ΔE_{DMF} (ZPE) -3200.253819
ΔG_{DMF} -3200.297968

6	-2.089051	-0.955728	0.004486
1	-1.522985	-0.796783	-0.929807
1	-1.524920	-0.793039	0.938852
1	-2.515381	-1.954993	0.005714
35	-3.578941	0.339452	-0.000031
46	0.315840	-0.299757	-0.001959
15	2.511956	0.149923	0.000578
6	3.121984	1.294668	-1.322049
1	4.203037	1.452676	-1.233300
1	2.900389	0.870138	-2.305128
1	2.609949	2.257288	-1.238615
6	3.189436	0.955147	1.525046
1	4.265431	1.138408	1.424920
1	2.677393	1.906356	1.694776
1	3.013661	0.309700	2.390084
6	3.659607	-1.289778	-0.198659
1	4.704521	-0.959068	-0.185732
1	3.498016	-2.002824	0.614429
1	3.454004	-1.794558	-1.146615

TS S_N22

ΔE_{DMF} -3200.38380535
ΔE_{DMF}(ZPE) -3200.235067
ΔG_{DMF} -3200.279497

6	1.706861	-0.034521	0.007579
1	1.736244	-0.786589	-0.777613
1	1.733188	-0.341977	1.050775
1	1.714634	1.023425	-0.250032
35	4.153667	0.010729	-0.000409
46	-0.426313	-0.010540	-0.002542
15	-2.794139	0.006491	-0.000308
6	-3.634611	-1.136803	-1.191598
1	-4.724881	-1.059310	-1.112223
1	-3.331075	-0.888317	-2.212716
1	-3.332483	-2.167544	-0.984610
6	-3.622019	-0.447985	1.593805
1	-4.713103	-0.413165	1.497088
1	-3.320253	-1.457346	1.888303
1	-3.309551	0.246602	2.378888
6	-3.615295	1.619703	-0.395246
1	-4.706756	1.525936	-0.366518
1	-3.301397	2.376701	0.329314
1	-3.310051	1.951158	-1.392019

Product S_N22

ΔE_{DMF} -3200.39431638
ΔE_{DMF}(ZPE) -3200.244833
ΔG_{DMF} -3200.289117

35	-5.474996	-0.042382	-0.000786
15	3.349809	-0.040352	-0.000245
46	0.861538	0.074478	-0.000952
6	4.227988	1.475359	-0.582087
1	3.960062	2.320819	0.057863
1	5.313460	1.335434	-0.556363
1	3.920146	1.705289	-1.605953
6	4.058311	-1.371142	-1.064511
1	3.751311	-1.212101	-2.102171
1	5.151535	-1.376977	-1.010024
1	3.677794	-2.342818	-0.736391
6	4.119507	-0.365549	1.645821
1	5.210072	-0.419877	1.565980
1	3.849776	0.435604	2.339614
1	3.741797	-1.310952	2.045628
6	-1.149910	0.119986	0.008344
1	-1.451502	-0.047877	1.048203
1	-1.440954	1.110606	-0.358122
1	-1.471896	-0.686427	-0.658667

2.2.3.4 PPh_3

$PdPPh_3$

ΔE_{DMF} -1164.24794548
ΔE_{DMF}(ZPE) -1163.972603
ΔG_{DMF} -1164.022441

15	-0.000236	0.000317	0.366595
6	-1.642235	-0.347064	-0.423606
6	0.521538	1.593610	-0.427798
6	1.120129	-1.248615	-0.424499
6	1.266880	-2.496378	0.206133
6	2.081969	-3.484428	-0.347588
6	2.778119	-3.234093	-1.534068
6	2.648371	-1.994886	-2.164423
6	1.821898	-1.008934	-1.616608
1	0.743250	-2.684027	1.141054
1	2.182108	-4.444213	0.152040
1	3.421786	-3.998417	-1.960683
1	3.188850	-1.791856	-3.085092
1	1.727056	-0.052018	-2.120682
6	-0.059230	2.097944	-1.602086
6	0.382477	3.306199	-2.150533
6	1.414346	4.021004	-1.539176
6	2.001743	3.526632	-0.370494
6	1.552304	2.327945	0.184497
1	-0.858892	1.551284	-2.092414
1	-0.081300	3.685410	-3.057225
1	1.755540	4.959884	-1.966461
1	2.801391	4.079710	0.114813
1	1.994358	1.956879	1.106657
6	-2.793964	0.171569	0.193817
6	-4.057582	-0.042379	-0.358073
6	-4.192378	-0.794930	-1.528838
6	-3.057011	-1.324413	-2.145311
6	-1.789200	-1.099256	-1.599897
1	-2.693054	0.737620	1.117384
1	-4.936736	0.368195	0.131192
1	-5.176635	-0.971769	-1.953631
1	-3.153692	-1.913431	-3.053435
1	-0.916016	-1.514239	-2.093887
46	0.000359	0.004545	2.565495

PPh_3

ΔE_{DMF} -1036.29059399
ΔE_{DMF}(ZPE) -1036.016277
ΔG_{DMF} -1036.062357

15	-0.000806	0.000258	-1.196993
6	-1.640448	-0.342479	-0.403969
6	-2.783265	0.117524	-1.082149
6	-1.811831	-1.041314	0.802492
6	-4.060320	-0.096249	-0.560160
1	-2.672521	0.643707	-2.027885
6	-3.090649	-1.264928	1.319566
1	-0.945413	-1.412085	1.342319
6	-4.216679	-0.790603	0.642376
1	-4.931547	0.269329	-1.097015
1	-3.205633	-1.808143	2.253871
1	-5.210136	-0.966310	1.045873
6	1.115424	-1.246718	-0.401652
6	1.777056	-1.056152	0.822724
6	1.316951	-2.453957	-1.093647
6	2.608390	-2.050635	1.344404
1	1.644105	-0.128677	1.372078
6	2.139623	-3.451974	-0.567797
1	0.828948	-2.612102	-2.053016
6	2.788956	-3.251142	0.653069
1	3.113494	-1.886912	2.292706
1	2.281206	-4.379684	-1.115686
1	3.436814	-4.022734	1.059943
6	0.522917	1.590037	-0.401656
6	1.496992	2.346950	-1.076597
6	0.002100	2.088485	0.803885
6	1.953997	3.557208	-0.552013
1	1.898081	1.987532	-2.021882
6	0.451631	3.305188	1.323706
1	-0.756078	1.526259	1.341174
6	1.430097	4.040135	0.650020
1	2.709761	4.126593	-1.086345
1	0.037744	3.676791	2.257433
1	1.777626	4.986318	1.055717

Adduct Conc2

ΔE_{DMF} -3775.59603801
ΔE_{DMF}(ZPE) -3775.282705
ΔG_{DMF} -3775.342706

6	4.932827	-1.339865	0.004824
1	4.610117	-1.847561	-0.899695
1	6.005503	-1.162614	0.016309
1	4.590074	-1.842733	0.904624
15	-0.677893	0.000066	-0.000956
46	1.568339	0.118932	-0.013149
35	4.080220	0.460702	-0.009236
6	-1.428389	-0.486108	1.621169
6	-0.729779	-1.413614	2.413648
6	-2.648751	0.022199	2.093749
6	-1.245588	-1.835540	3.639741
1	0.227608	-1.796132	2.066335
6	-3.158820	-0.391895	3.327991
1	-3.203870	0.744766	1.503204
6	-2.461533	-1.322510	4.101214
1	-0.693928	-2.555050	4.238675
1	-4.102589	0.013862	3.682302
1	-2.859599	-1.642065	5.060323
6	-1.544275	1.582284	-0.419666
6	-2.731429	1.636725	-1.166531
6	-0.978194	2.784071	0.040611
6	-3.339281	2.865156	-1.443256
1	-3.183995	0.721640	-1.536081
6	-1.592201	4.008533	-0.225675
1	-0.047265	2.754037	0.602505
6	-2.774087	4.051745	-0.971543
1	-4.255744	2.891486	-2.026564
1	-1.143255	4.928122	0.139795
1	-3.247804	5.005242	-1.188032
6	-1.405769	-1.217346	-1.192808
6	-0.770828	-1.379532	-2.436660
6	-2.551093	-1.979565	-0.914544
6	-1.277023	-2.270186	-3.384336
1	0.128900	-0.808081	-2.654387
6	-3.050474	-2.880631	-1.859923
1	-3.055977	-1.874006	0.040796
6	-2.417472	-3.025914	-3.096110
1	-0.775741	-2.381602	-4.341972
1	-3.935722	-3.466623	-1.627985
1	-2.806662	-3.727154	-3.829066

TS Conc2

ΔE_{DMF} -3775.56992503
ΔE_{DMF} (ZPE) -3775.258735
ΔG_{DMF} -3775.314078

6	-3.564019	1.872266	0.016358
1	-4.100050	2.149659	-0.883883
1	-4.088798	2.113631	0.933502
1	-2.531727	2.324029	0.017281
15	0.624994	0.048274	0.000511
46	-1.589787	0.651672	-0.001809
35	-4.003105	-0.289367	-0.029819
6	1.175607	-0.813971	1.540722
6	0.602565	-0.413489	2.760148
6	2.132988	-1.840656	1.547066
6	0.989137	-1.014016	3.959249
1	-0.154178	0.368120	2.763862
6	2.510922	-2.449189	2.747514
1	2.584844	-2.169882	0.616189
6	1.943062	-2.035959	3.954710
1	0.538980	-0.691355	4.894059
1	3.250521	-3.245184	2.736505
1	2.237852	-2.510778	4.886379
6	1.116661	-1.113702	-1.353570
6	2.349610	-1.042085	-2.020773
6	0.200511	-2.112063	-1.728292
6	2.658402	-1.950138	-3.038114
1	3.070941	-0.276825	-1.751231
6	0.514804	-3.024865	-2.735933
1	-0.764585	-2.167794	-1.230566
6	1.744594	-2.943544	-3.395897
1	3.614936	-1.879144	-3.548733
1	-0.203637	-3.791859	-3.012004
1	1.986295	-3.647364	-4.187451
6	1.825781	1.446579	-0.171266
6	1.468242	2.520765	-1.004386
6	3.066065	1.483878	0.485255
6	2.335011	3.598732	-1.188923
1	0.501701	2.511816	-1.503533
6	3.928428	2.570195	0.309346
1	3.361992	0.667865	1.137564
6	3.567072	3.627071	-0.528907
1	2.044449	4.419585	-1.838901
1	4.883215	2.586976	0.827842
1	4.238552	4.470468	-0.663523

Product Conc2

ΔE_{DMF} -3775.61058859
ΔE_{DMF}(ZPE) -3775.298911
ΔG_{DMF} -3775.355061

6	3.170522	2.490219	0.023427
1	3.766860	2.405020	0.936133
1	3.806508	2.386360	-0.859229
1	2.608296	3.437766	0.001361
15	-0.522123	-0.026114	0.005652
46	1.613105	1.188522	0.011844
35	3.269101	-0.643875	0.014922
6	-0.854159	-1.204263	-1.364882
6	-0.150240	-1.034756	-2.569080
6	-1.783521	-2.251496	-1.257830
6	-0.381542	-1.887994	-3.649943
1	0.581182	-0.235321	-2.658230
6	-2.008104	-3.107231	-2.338516
1	-2.331544	-2.400672	-0.332376
6	-1.309834	-2.925895	-3.535376
1	0.168452	-1.746624	-4.576064
1	-2.728889	-3.914648	-2.244168
1	-1.485737	-3.593831	-4.373883
6	-0.994077	-0.924181	1.540081
6	-2.291596	-0.885588	2.076097
6	-0.004315	-1.678631	2.194309
6	-2.593590	-1.592542	3.242582
1	-3.065923	-0.301253	1.588165
6	-0.313074	-2.390790	3.354881
1	1.006335	-1.704163	1.794975
6	-1.606915	-2.347030	3.881972
1	-3.600396	-1.553536	3.649098
1	0.458835	-2.972377	3.851152
1	-1.844335	-2.895621	4.789128
6	-1.793216	1.296173	-0.171362
6	-1.740840	2.370658	0.737771
6	-2.739087	1.328268	-1.206875
6	-2.622715	3.444965	0.618411
1	-1.010595	2.365377	1.544473
6	-3.616359	2.410453	-1.327878
1	-2.793578	0.512719	-1.921025
6	-3.561221	3.468300	-0.418096
1	-2.573644	4.263983	1.330499
1	-4.344182	2.422662	-2.134409
1	-4.243849	4.307621	-0.515637

Adduct Conc1

ΔE_{DMF} -3775.59607804
ΔE_{DMF}(ZPE) -3775.282646
ΔG_{DMF} -3775.341998

6	4.935946	1.334383	0.013801
1	4.598025	1.839295	0.914331
1	6.008336	1.155174	0.020901
1	4.610295	1.841368	-0.890082
15	-0.677210	-0.001069	0.004153
46	1.568663	-0.121871	-0.000909
35	4.079824	-0.464742	0.006281
6	-1.374232	1.575775	-0.673539
6	-0.672963	2.767694	-0.420812
6	-2.561836	1.635306	-1.419548
6	-1.154692	3.990640	-0.889920
1	0.257999	2.729814	0.140757
6	-3.037748	2.859580	-1.898609
1	-3.117724	0.726774	-1.630552
6	-2.338065	4.038578	-1.633012
1	-0.602064	4.903301	-0.683977
1	-3.956591	2.889098	-2.477995
1	-2.709058	4.988822	-2.006969
6	-1.526839	-1.308806	-0.995457
6	-2.723544	-1.927856	-0.602152
6	-0.931399	-1.696489	-2.208856
6	-3.311584	-2.909501	-1.405997
1	-3.199785	-1.647878	0.332370
6	-1.525918	-2.666609	-3.016463
1	0.007068	-1.237951	-2.512749
6	-2.717242	-3.278405	-2.614355
1	-4.235639	-3.383070	-1.085536
1	-1.054240	-2.952331	-3.952743
1	-3.175570	-4.041669	-3.237085
6	-1.476424	-0.141242	1.669357
6	-0.876526	-0.987684	2.617819
6	-2.644219	0.551777	2.025211
6	-1.437928	-1.148997	3.885332
1	0.039641	-1.513588	2.358244
6	-3.199152	0.399141	3.299324
1	-3.122883	1.213839	1.310138
6	-2.599944	-0.452410	4.230086
1	-0.962881	-1.809108	4.605965
1	-4.100928	0.945904	3.561431
1	-3.032351	-0.568951	5.219982

TS Conc1

DE -3775.57181178
DE(ZPE) -3775.260233
DG -3775.316345

6	3.273366	1.690298	-0.255011
1	3.073062	2.062319	0.743189
1	4.240634	1.969818	-0.651633
1	2.465143	1.809530	-0.970688
15	-0.626858	-0.035057	0.005519
46	1.644245	-0.288983	0.036739
35	4.089904	-0.459114	0.073288
6	-1.188649	1.717058	-0.163793
6	-0.547956	2.687432	0.628288
6	-2.190547	2.127412	-1.055922
6	-0.911208	4.031541	0.540517
1	0.241128	2.387113	1.314037
6	-2.544359	3.477432	-1.152088
1	-2.697382	1.398064	-1.679886
6	-1.909281	4.430608	-0.354410
1	-0.409561	4.767213	1.163195
1	-3.319478	3.779773	-1.850997
1	-2.185939	5.478374	-0.430887
6	-1.480393	-0.924922	-1.370587
6	-2.800185	-1.396078	-1.278421
6	-0.765699	-1.138544	-2.561496
6	-3.391698	-2.059723	-2.356445
1	-3.368372	-1.250689	-0.364454
6	-1.360867	-1.793834	-3.641117
1	0.264437	-0.796611	-2.632383
6	-2.675131	-2.257599	-3.539495
1	-4.412551	-2.421690	-2.270052
1	-0.795254	-1.950655	-4.555488
1	-3.136591	-2.775684	-4.375556
6	-1.501229	-0.633755	1.519268
6	-0.993207	-1.777675	2.159013
6	-2.641548	-0.009955	2.050335
6	-1.620157	-2.296215	3.292880
1	-0.098167	-2.256487	1.767867
6	-3.261798	-0.524198	3.192847
1	-3.046526	0.879485	1.576680
6	-2.755423	-1.668293	3.813619
1	-1.216849	-3.182548	3.774910
1	-4.141857	-0.029605	3.594822
1	-3.239139	-2.065612	4.701593

Product Conc1

ΔE_{DMF} -3775.63813167
ΔE_{DMF}(ZPE) -3775.324782
ΔG_{DMF} -3775.381104

6	-1.563714	1.375925	-1.732996
1	-2.146227	0.903276	-2.528189
1	-2.062949	2.276190	-1.364469
1	-0.555095	1.610138	-2.072353
46	-1.638926	0.087943	-0.164693
15	0.640049	0.002148	-0.018734
35	-4.165187	-0.012258	-0.070429
6	1.520045	1.610997	-0.075518
6	2.788575	1.760883	-0.656432
6	0.886773	2.730772	0.491894
6	3.414579	3.010211	-0.662117
1	3.290022	0.910101	-1.106152
6	1.519604	3.974042	0.491992
1	-0.104910	2.628215	0.925240
6	2.784134	4.115617	-0.087126
1	4.394837	3.116254	-1.117777
1	1.021393	4.831750	0.934525
1	3.273050	5.085528	-0.094764
6	1.469254	-1.105511	-1.225198
6	2.686868	-1.737419	-0.918331
6	0.878850	-1.325146	-2.480265
6	3.305729	-2.563752	-1.857923
1	3.148844	-1.592114	0.053763
6	1.503400	-2.149996	-3.418026
1	-0.073209	-0.861554	-2.719296
6	2.716728	-2.768973	-3.108704
1	4.245646	-3.048609	-1.610493
1	1.037203	-2.313569	-4.385314
1	3.198959	-3.414923	-3.836734
6	1.000340	-0.733612	1.627078
6	1.743856	-0.065697	2.611577
6	0.450557	-1.997120	1.917972
6	1.940309	-0.656060	3.863281
1	2.172161	0.909948	2.406136
6	0.651501	-2.581608	3.168210
1	-0.129459	-2.526324	1.165654
6	1.396170	-1.911116	4.143603
1	2.522468	-0.132974	4.616493
1	0.226255	-3.558299	3.380229
1	1.551063	-2.366211	5.117572

Adduct S_N21

ΔE_{DMF} -3775.57951460
ΔE_{DMF}(ZPE) -3775.266492
ΔG_{DMF} -3775.329396

6	-3.644569	-0.050855	-0.362691
1	-3.242649	-0.149566	0.641583
1	-3.409688	-0.915689	-0.977653
1	-3.328855	0.875692	-0.835075
35	-5.624122	0.024168	-0.192127
15	0.987530	0.005908	-0.204631
46	-0.516869	0.055163	-1.811013
6	0.426346	-0.739369	1.398426
6	-0.450106	-1.837550	1.345045
6	0.829732	-0.260705	2.654916
6	-0.902236	-2.448544	2.515792
1	-0.784071	-2.205674	0.377667
6	0.366520	-0.865364	3.828000
1	1.504893	0.586601	2.724134
6	-0.497696	-1.959820	3.762101
1	-1.577209	-3.297977	2.454872
1	0.684663	-0.478638	4.792432
1	-0.857622	-2.427038	4.674515
6	1.652388	1.659718	0.307412
6	2.983098	1.863507	0.706240
6	0.775375	2.758162	0.296034
6	3.423584	3.134755	1.086749
1	3.680612	1.031516	0.719134
6	1.212446	4.024435	0.687331
1	-0.251430	2.615331	-0.033155
6	2.540185	4.216306	1.080979
1	4.457891	3.276662	1.388365
1	0.520466	4.862232	0.674081
1	2.884746	5.203704	1.375559
6	2.522114	-0.955781	-0.605788
6	3.045132	-0.846833	-1.906617
6	3.178582	-1.784612	0.317328
6	4.202145	-1.536183	-2.270399
1	2.533160	-0.223517	-2.636723
6	4.330675	-2.486380	-0.052329
1	2.793247	-1.887480	1.326981
6	4.846326	-2.362107	-1.343658
1	4.594209	-1.438060	-3.279118
1	4.823735	-3.128248	0.672818
1	5.740946	-2.908567	-1.629109

TS S_N21

ΔE_{DMF} -3775.57249081
ΔE_{DMF}(ZPE) -3775.260530
ΔG_{DMF} -3775.320216

6	-2.741294	0.036289	-0.780146
1	-2.340665	0.094706	0.218104
1	-2.750465	-0.926992	-1.273123
1	-2.806109	0.941440	-1.368913
35	-4.961479	0.007018	-0.172271
15	0.852166	0.003829	-0.178861
46	-0.528276	0.007212	-1.930851
6	0.207559	-0.838616	1.335650
6	-0.463886	-2.064029	1.173376
6	0.339238	-0.305093	2.626609
6	-0.978825	-2.744815	2.276807
1	-0.590460	-2.479514	0.176238
6	-0.188517	-0.983076	3.730456
1	0.852101	0.639466	2.776756
6	-0.845679	-2.202410	3.559363
1	-1.492826	-3.691348	2.134364
1	-0.082933	-0.554503	4.723276
1	-1.256576	-2.726217	4.417796
6	1.363620	1.679053	0.415228
6	2.622318	1.928675	0.986011
6	0.450001	2.739970	0.295743
6	2.955726	3.210716	1.430924
1	3.345929	1.125050	1.082740
6	0.781095	4.017879	0.749556
1	-0.518998	2.561218	-0.163510
6	2.036237	4.256094	1.316264
1	3.934618	3.390166	1.866959
1	0.063238	4.827629	0.651969
1	2.298182	5.252315	1.661554
6	2.457727	-0.851209	-0.510319
6	3.045350	-0.688152	-1.777124
6	3.111395	-1.646596	0.443859
6	4.265094	-1.295449	-2.077634
1	2.539363	-0.087096	-2.529609
6	4.328197	-2.263053	0.137014
1	2.673423	-1.788530	1.426950
6	4.907893	-2.087365	-1.121076

1	4.708335	-1.158806	-3.060162
1	4.821299	-2.878588	0.884377
1	5.852988	-2.568093	-1.357574

Product S_N21

ΔE_{DMF} -3775.60679930
ΔE_{DMF} (ZPE) -3775.293728
ΔG_{DMF} -3775.351449

6	1.897453	-0.271483	-0.805936
1	2.002698	0.473135	-0.015825
1	2.621934	-0.085775	-1.610336
1	1.985474	-1.286452	-0.411841
35	6.345695	-0.038135	-0.342768
15	-1.082503	-0.015057	-0.014329
46	0.196541	-0.114807	-1.858016
6	-0.957018	-1.412016	1.165041
6	0.160771	-1.483908	2.017035
6	-1.924366	-2.427972	1.212607
6	0.302546	-2.553331	2.900346
1	0.914572	-0.702821	2.006026
6	-1.774002	-3.497632	2.099101
1	-2.796730	-2.388855	0.569212
6	-0.663106	-3.563562	2.941692
1	1.166727	-2.594966	3.556663
1	-2.531947	-4.274758	2.131418
1	-0.550213	-4.395601	3.630468
6	-2.787587	0.002711	-0.691292
6	-3.733031	0.957007	-0.280869
6	-3.138936	-0.935689	-1.680950
6	-5.011152	0.961723	-0.843019
1	-3.477339	1.692018	0.474571
6	-4.419418	-0.926165	-2.235442
1	-2.419201	-1.677982	-2.017340
6	-5.356154	0.022724	-1.818120
1	-5.736049	1.701965	-0.517610
1	-4.681276	-1.657664	-2.994045
1	-6.350849	0.032051	-2.253927
6	-0.873311	1.504619	0.979423
6	-0.282865	2.634149	0.390704
6	-1.341024	1.576756	2.303145
6	-0.165457	3.822054	1.113791
1	0.088186	2.578114	-0.628883
6	-1.220003	2.767558	3.021061
1	-1.795448	0.710375	2.773722
6	-0.633207	3.889113	2.428388
1	0.296316	4.689855	0.652376
1	-1.583057	2.816762	4.043331
1	-0.537252	4.812353	2.992330

Adduct S_N22

ΔE_{DMF} -3775.58016053
ΔE_{DMF}(ZPE) -3775.267452
ΔG_{DMF} -3775.324840

6	3.754067	-1.044182	0.467873
1	3.209014	-0.526342	1.274083
1	3.178513	-1.231610	-0.455959
1	4.160165	-1.980225	0.841392
35	5.267912	0.117085	-0.036505
46	1.343570	-0.421756	0.222832
15	-0.857295	-0.033641	0.019788
6	-1.830757	-0.160467	1.588646
6	-1.440658	-1.128112	2.531620
6	-2.937000	0.656319	1.874648
6	-2.147748	-1.284136	3.725026
1	-0.575529	-1.754812	2.324773
6	-3.639276	0.503326	3.074283
1	-3.253342	1.414182	1.164099
6	-3.246995	-0.465498	4.000123
1	-1.836441	-2.038321	4.442553
1	-4.491448	1.144336	3.282915
1	-3.791053	-0.579425	4.933585
6	-1.274149	1.654404	-0.609933
6	-2.314123	1.904421	-1.518765
6	-0.494259	2.733572	-0.157044
6	-2.568552	3.206293	-1.962135
1	-2.924553	1.084899	-1.887562
6	-0.757948	4.033354	-0.590444
1	0.329565	2.546675	0.528689
6	-1.796020	4.272110	-1.496518
1	-3.371970	3.383644	-2.671879
1	-0.147002	4.856801	-0.230879
1	-1.993216	5.281836	-1.845689
6	-1.738620	-1.170777	-1.144091
6	-1.046006	-1.608909	-2.284959
6	-3.055727	-1.613248	-0.939317
6	-1.658565	-2.458505	-3.207015
1	-0.018865	-1.286784	-2.439979
6	-3.663366	-2.475307	-1.857361
1	-3.610895	-1.292838	-0.063633
6	-2.969146	-2.896332	-2.993080
1	-1.110252	-2.785266	-4.086241
1	-4.680966	-2.814349	-1.683442
1	-3.444354	-3.564917	-3.705571

TS S_N22

ΔE_{DMF} -3775.55953809
ΔE_{DMF}(ZPE) -3775.249397
ΔG_{DMF} -3775.309670

6	-3.489523	-0.010098	0.068668
1	-3.527549	-0.949596	0.614453
1	-3.489277	-0.011841	-1.019472
1	-3.519260	0.930800	0.612982
35	-5.933521	0.003548	-0.007679
46	-1.356182	-0.003056	0.040750
15	1.011271	0.000351	0.001104
6	1.770258	1.626522	-0.441112
6	1.097304	2.426738	-1.380785
6	2.968534	2.099133	0.116760
6	1.618299	3.662742	-1.766181
1	0.158168	2.079163	-1.806417
6	3.483272	3.342548	-0.261500
1	3.501065	1.501106	0.850034
6	2.812338	4.124347	-1.204454
1	1.087578	4.268494	-2.495499
1	4.409759	3.697505	0.181558
1	3.213943	5.090735	-1.496172
6	1.802578	-0.439697	1.611997
6	3.004022	-1.158464	1.714608
6	1.153161	-0.031484	2.789851
6	3.545107	-1.456712	2.968484
1	3.518550	-1.490038	0.817721
6	1.700107	-0.320361	4.040962
1	0.212324	0.511105	2.722368
6	2.897221	-1.036448	4.132283
1	4.473919	-2.016876	3.033128
1	1.187510	0.004176	4.942303
1	3.319313	-1.270381	5.105622
6	1.760032	-1.185517	-1.202409
6	1.096849	-2.407058	-1.412171
6	2.941540	-0.925073	-1.914283
6	1.611580	-3.353378	-2.299452
1	0.169928	-2.612186	-0.880320
6	3.449750	-1.869000	-2.811461
1	3.466365	0.015182	-1.774269
6	2.789026	-3.084391	-3.003370
1	1.088644	-4.294014	-2.448591
1	4.363248	-1.652353	-3.358491
1	3.185580	-3.815928	-3.701843

Product S_N22

ΔE_{DMF} -3775.56920452
ΔE_{DMF}(ZPE) -3775.257978
ΔG_{DMF} -3775.317527

6	3.119119	-0.099436	0.243260
1	3.444546	0.154977	-0.770953
1	3.410689	-1.113006	0.537743
1	3.413035	0.653788	0.981836
35	7.454924	-0.008154	0.024027
46	1.107586	-0.077785	0.187118
15	-1.369208	-0.006196	0.018758
6	-2.242595	0.146874	1.627837
6	-1.695278	-0.521764	2.736721
6	-3.414353	0.901896	1.792967
6	-2.316915	-0.447552	3.984055
1	-0.782360	-1.102272	2.622386
6	-4.029837	0.980029	3.044700
1	-3.845091	1.431262	0.948455
6	-3.484304	0.305219	4.139576
1	-1.886319	-0.969872	4.833583
1	-4.935780	1.567917	3.162017
1	-3.964635	0.368958	5.111786
6	-1.943222	1.420174	-0.990125
6	-3.029089	1.342676	-1.876075
6	-1.243099	2.634477	-0.869202
6	-3.410640	2.461102	-2.621739
1	-3.575963	0.411383	-1.988143
6	-1.632338	3.751415	-1.609770
1	-0.391897	2.709737	-0.194964
6	-2.715889	3.665501	-2.488664
1	-4.251784	2.389062	-3.305420
1	-1.085444	4.684204	-1.506153
1	-3.014092	4.532794	-3.070730
6	-2.075121	-1.501607	-0.785830
6	-1.333535	-2.104926	-1.817286
6	-3.300299	-2.068908	-0.403030
6	-1.814760	-3.246372	-2.459827
1	-0.378512	-1.681192	-2.120056
6	-3.775620	-3.216220	-1.043485
1	-3.882310	-1.619406	0.395693
6	-3.035928	-3.804873	-2.071798
1	-1.233535	-3.702360	-3.256200
1	-4.724344	-3.648059	-0.737579
1	-3.407163	-4.697699	-2.566790