Supporting Information for

A Computational Study of Mechanism for the Transmetalation of 2-Trimethylstannylbuta-1,3-diene with $SnCl_4$

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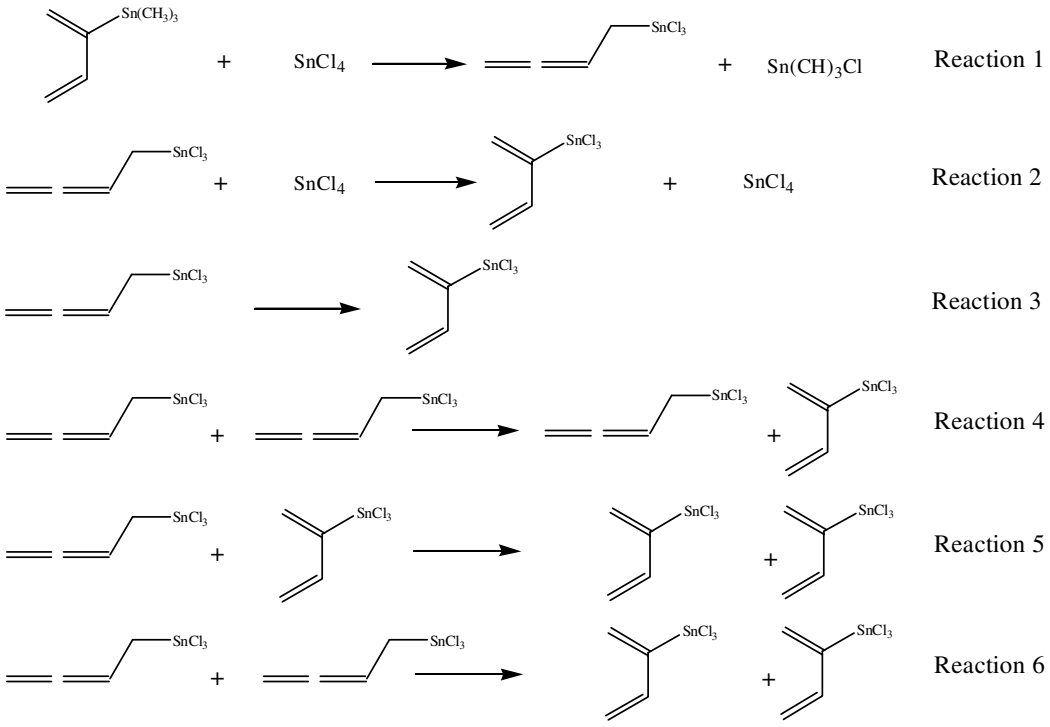

1. SnCl4

Z-Matrix
Sn
Cl,1,B1
Cl,1,B1,2,A1
Cl,1,B1,2,A1,3,D1,0
Cl,1,B1,2,A1,3,D2,0
Variables:

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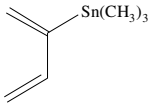
B1=2.32604131
A1=109.47122063
Constants:
D1=120.
D2=-120.

Zero-point correction=	0.004548 (Hartree/Particle)
Thermal correction to Energy=	0.012352
Thermal correction to Enthalpy=	0.013296
Thermal correction to Gibbs Free Energy=	-0.028794
Sum of electronic and zero-point Energies=	-1844.319926
Sum of electronic and thermal Energies=	-1844.312122
Sum of electronic and thermal Enthalpies=	-1844.311178
Sum of electronic and thermal Free Energies=	-1844.353268



2. (RE1)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.267308	0.019831	-2.207137
2	6	0	1.261246	0.032069	-0.863357
3	6	0	2.515718	0.013220	-0.085648
4	6	0	3.556245	-0.797833	-0.319369
5	50	0	-0.614646	0.070354	0.214493
6	6	0	-2.217820	0.244465	-1.213349
7	6	0	-0.826372	-1.745133	1.356978
8	6	0	-0.621782	1.767230	1.544916
9	1	0	2.199943	0.047127	-2.771622
10	1	0	0.353686	-0.003389	-2.796754
11	1	0	2.572189	0.695822	0.764770
12	1	0	3.533978	-1.529251	-1.122665
13	1	0	4.452478	-0.763525	0.293150
14	1	0	-2.146520	1.186937	-1.762946
15	1	0	-2.192003	-0.578357	-1.932976
16	1	0	-3.183772	0.218467	-0.701040
17	1	0	-1.727491	-1.708402	1.975795
18	1	0	-0.899051	-2.609505	0.691291
19	1	0	0.037118	-1.889453	2.011956

20	1	0	-0.505667	2.696898	0.981150
21	1	0	-1.564443	1.815488	2.097517
22	1	0	0.194602	1.700332	2.269519

Zero-point correction= 0.183751 (Hartree/Particle)
Thermal correction to Energy= 0.197541
Thermal correction to Enthalpy= 0.198485
Thermal correction to Gibbs Free Energy= 0.141594
Sum of electronic and zero-point Energies= -278.364893
Sum of electronic and thermal Energies= -278.351104
Sum of electronic and thermal Enthalpies= -278.350160
Sum of electronic and thermal Free Energies= -278.407051

3.molecular complex IN1a (SnCl4 + RE1)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.037114	2.468184	-0.977654
2	6	0	-2.555369	1.572855	-0.097904
3	6	0	-1.453700	1.919565	0.820374
4	6	0	-0.357068	2.618995	0.489593
5	50	0	2.739825	-0.121738	-0.033244
6	17	0	4.557555	-1.540244	-0.372120
7	17	0	3.554225	1.987488	0.517640
8	17	0	1.481469	-0.979613	1.725521
9	50	0	-3.442064	-0.400137	0.019298
10	17	0	1.517135	-0.031013	-2.006353
11	6	0	-5.130600	-0.452441	-1.315872
12	6	0	-2.010241	-1.906672	-0.548515
13	6	0	-4.083816	-0.739238	2.049743
14	1	0	-2.662380	3.491644	-1.012328
15	1	0	-3.828975	2.227269	-1.682948
16	1	0	-1.541255	1.556156	1.845962
17	1	0	-0.195780	2.974114	-0.524768
18	1	0	0.401920	2.865296	1.226519
19	1	0	-5.843516	0.340165	-1.073243
20	1	0	-4.812138	-0.325646	-2.354194
21	1	0	-5.646015	-1.413579	-1.233636
22	1	0	-2.475108	-2.896732	-0.533306

23	1	0	-1.633194	-1.716491	-1.556893
24	1	0	-1.162177	-1.913471	0.141082
25	1	0	-4.836893	-0.002819	2.343127
26	1	0	-4.520217	-1.737065	2.150475
27	1	0	-3.241389	-0.665107	2.743164

Zero-point correction= 0.188962 (Hartree/Particle)
Thermal correction to Energy= 0.212870
Thermal correction to Enthalpy= 0.213814
Thermal correction to Gibbs Free Energy= 0.125845
Sum of electronic and zero-point Energies= -2122.685856
Sum of electronic and thermal Energies= -2122.661948
Sum of electronic and thermal Enthalpies= -2122.661004
Sum of electronic and thermal Free Energies= -2122.748973

4. transition state for reaction 1 (TS1)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.502000	1.628251	-3.111447
2	6	0	0.497259	1.628817	-1.789657
3	6	0	1.155565	1.630603	-0.605226
4	6	0	2.044069	0.563373	-0.163322
5	50	0	1.227386	-1.264018	0.848254
6	17	0	1.616084	-3.397563	-0.108013
7	17	0	3.273634	-1.327670	2.182797
8	17	0	-0.189446	-1.039065	2.745734
9	50	0	-1.874491	1.726036	-0.944978
10	17	0	-0.876446	-1.149631	-0.678889
11	6	0	-2.936342	0.851432	-2.582482
12	6	0	-2.474339	1.330035	1.064452
13	6	0	-1.730745	3.873795	-1.151408
14	1	0	1.372968	1.997592	-3.651826
15	1	0	-0.348913	1.319525	-3.710082
16	1	0	0.966410	2.447052	0.094980
17	1	0	2.562424	0.090685	-1.002815
18	1	0	2.744797	0.903408	0.599075
19	1	0	-3.108573	1.596945	-3.362366
20	1	0	-2.381992	0.001935	-2.983385

21	1	0	-3.897886	0.484244	-2.213756
22	1	0	-3.181111	2.110482	1.363524
23	1	0	-2.941034	0.346811	1.120997
24	1	0	-1.624678	1.337595	1.748295
25	1	0	-1.523887	4.157414	-2.185176
26	1	0	-2.684693	4.316218	-0.844632
27	1	0	-0.948426	4.288154	-0.509802

	1	2	3
	?A	?A	?A
Frequencies --	-129.9327	23.8175	36.7678

Zero-point correction= 0.189235 (Hartree/Particle)
Thermal correction to Energy= 0.211728
Thermal correction to Enthalpy= 0.212673
Thermal correction to Gibbs Free Energy= 0.133704
Sum of electronic and zero-point Energies= -2122.656097
Sum of electronic and thermal Energies= -2122.633604
Sum of electronic and thermal Enthalpies= -2122.632660
Sum of electronic and thermal Free Energies= -2122.711629

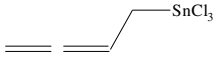
5. molecular complex IN1b (PR1a + PR1b)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.659048	1.369388	-1.918061
2	6	0	4.246473	0.294502	-1.303739
3	6	0	3.833036	-0.790577	-0.690788
4	6	0	2.413648	-1.268602	-0.711443
5	50	0	1.432171	-0.864941	1.180805
6	17	0	-0.368352	-2.259117	1.796572
7	17	0	3.007209	-1.151500	2.923330
8	17	0	0.691791	1.368784	1.433294
9	50	0	-2.729345	1.043037	-1.308327
10	17	0	-0.943881	-0.513720	-1.827220
11	6	0	-4.206499	0.603708	-2.795342
12	6	0	-3.333083	0.558687	0.683081
13	6	0	-1.833602	2.972556	-1.529648
14	1	0	5.003673	1.338160	-2.949505

15	1	0	4.673539	2.336486	-1.419876
16	1	0	4.551832	-1.383286	-0.126105
17	1	0	1.797692	-0.771491	-1.461375
18	1	0	2.332468	-2.351942	-0.836131
19	1	0	-5.073347	1.259563	-2.671430
20	1	0	-3.791270	0.753196	-3.794471
21	1	0	-4.534286	-0.434135	-2.703342
22	1	0	-4.176136	1.189852	0.979482
23	1	0	-3.636566	-0.488664	0.739836
24	1	0	-2.504728	0.723224	1.374509
25	1	0	-1.459652	3.100218	-2.547943
26	1	0	-2.571359	3.753750	-1.324007
27	1	0	-1.002292	3.076698	-0.829455

Zero-point correction= 0.188790 (Hartree/Particle)
Thermal correction to Energy= 0.212994
Thermal correction to Enthalpy= 0.213938
Thermal correction to Gibbs Free Energy= 0.124933
Sum of electronic and zero-point Energies= -2122.711246
Sum of electronic and thermal Energies= -2122.687042
Sum of electronic and thermal Enthalpies= -2122.686098
Sum of electronic and thermal Free Energies= -2122.775104

6.  (PR1a)

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.304984
3	1	0	0.929042	0.000000	-0.566042
4	1	0	-0.927350	-0.000973	-0.568882
5	-1	0	-0.028052	-0.999178	1.275711
6	6	0	-0.004464	-0.003583	2.617449
7	1	0	0.005640	0.947176	3.149846
8	6	0	-0.010830	-1.251563	3.450192
9	1	0	-0.701089	-1.190380	4.296339
10	1	0	-0.238877	-2.145652	2.866074
11	50	0	1.930613	-1.612140	4.338373

12	17	0	3.566851	-2.079978	2.715091
13	17	0	2.677944	0.274631	5.531894
14	17	0	1.915965	-3.422546	5.850031

Zero-point correction= 0.077962 (Hartree/Particle)
Thermal correction to Energy= 0.089705
Thermal correction to Enthalpy= 0.090649
Thermal correction to Gibbs Free Energy= 0.035782
Sum of electronic and zero-point Energies= -1539.410353
Sum of electronic and thermal Energies= -1539.398609
Sum of electronic and thermal Enthalpies= -1539.397665
Sum of electronic and thermal Free Energies= -1539.452532

7. $Sn(CH_3)_3Cl$ (PR1b)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	-0.000857	-0.000093	-0.262380
2	17	0	0.008733	-0.000615	2.135990
3	6	0	2.062955	0.014498	-0.834863
4	6	0	-1.025267	-1.795437	-0.823440
5	6	0	-1.048862	1.782501	-0.819882
6	1	0	2.153325	-0.023779	-1.924463
7	1	0	2.547677	0.924008	-0.472990
8	1	0	2.577520	-0.849328	-0.408176
9	1	0	-2.045050	-1.784718	-0.432299
10	1	0	-1.066175	-1.881687	-1.913292
11	1	0	-0.505646	-2.667439	-0.420136
12	1	0	-0.541773	2.660014	-0.412619
13	1	0	-1.089480	1.872259	-1.909433
14	1	0	-2.068990	1.756419	-0.430331

Zero-point correction= 0.110150 (Hartree/Particle)
Thermal correction to Energy= 0.120259
Thermal correction to Enthalpy= 0.121204
Thermal correction to Gibbs Free Energy= 0.073239
Sum of electronic and zero-point Energies= -583.295237
Sum of electronic and thermal Energies= -583.285127

Sum of electronic and thermal Enthalpies= -583.284183
Sum of electronic and thermal Free Energies= -583.332147

8. molecular complex IN2a (PR1a + SnCl4)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.476797	-0.519646	-2.126197
2	6	0	1.621577	-0.107743	-0.894808
3	6	0	1.776706	0.304167	0.341417
4	6	0	2.907754	-0.123518	1.229208
5	50	0	2.251395	-1.564390	2.705903
6	17	0	1.574319	-3.586570	1.715250
7	17	0	3.940927	-2.088860	4.264755
8	17	0	0.411736	-0.753849	3.929590
9	50	0	-2.288251	1.607889	-2.481068
10	17	0	-0.801102	2.117602	-4.196629
11	17	0	-4.356761	2.551076	-2.971348
12	17	0	-2.536596	-0.695740	-2.292076
13	17	0	-1.513017	2.504822	-0.477215
14	1	0	1.929513	0.011904	-2.960643
15	1	0	0.903780	-1.414862	-2.358970
16	1	0	1.044799	0.992014	0.763377
17	1	0	3.713440	-0.613541	0.678389
18	1	0	3.322675	0.705811	1.808809

Zero-point correction= 0.082857 (Hartree/Particle)
Thermal correction to Energy= 0.104953
Thermal correction to Enthalpy= 0.105898
Thermal correction to Gibbs Free Energy= 0.016055
Sum of electronic and zero-point Energies= -3383.731386
Sum of electronic and thermal Energies= -3383.709289
Sum of electronic and thermal Enthalpies= -3383.708345
Sum of electronic and thermal Free Energies= -3383.798187

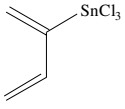
9.transition state for reaction 2 (TS2)

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.338306
3	-1	0	1.000000	0.000000	1.338306
4	6	0	0.261110	-0.977625	2.299137
5	6	0	-0.456343	-2.202186	2.364013
6	50	0	-2.415023	-1.991740	3.576380
7	17	0	-4.458647	-2.452063	2.518555
8	17	0	-2.068258	-4.184847	4.477482
9	17	0	-2.211798	-0.759701	5.558727
10	50	0	-0.634600	1.952386	2.349211
11	17	0	-1.190576	3.304438	0.516246
12	17	0	-1.429530	2.936346	4.330144
13	17	0	-2.859067	0.490070	2.334841
14	17	0	1.695072	2.303531	2.844132
15	1	0	0.500045	-0.797732	-0.547825
16	1	0	-0.401069	0.822696	-0.583845
17	1	0	0.936995	-0.725240	3.119419
18	1	0	-0.878670	-2.544114	1.415001
19	1	0	-0.004459	-2.982419	2.975031

	1	2	3
	?A	?A	?A
Frequencies --	-122.1143	12.5955	30.6608

Zero-point correction= 0.083911 (Hartree/Particle)
Thermal correction to Energy= 0.104107
Thermal correction to Enthalpy= 0.105051
Thermal correction to Gibbs Free Energy= 0.029194
Sum of electronic and zero-point Energies= -3383.690185
Sum of electronic and thermal Energies= -3383.669990
Sum of electronic and thermal Enthalpies= -3383.669045
Sum of electronic and thermal Free Energies= -3383.744902



10. (PR2)

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.338613
3	1	0	0.928620	0.000000	-0.561745
4	1	0	-0.924940	0.011726	-0.569347
5	6	0	-1.223577	-0.030062	2.156701
6	6	0	-2.284419	-0.821249	1.943756
7	1	0	-2.265140	-1.553383	1.138092
8	1	0	-3.182581	-0.787515	2.553274
9	50	0	-1.316396	1.306192	3.813035
10	17	0	-3.209923	0.858198	5.131614
11	17	0	-1.431234	3.572365	3.202917
12	17	0	0.581769	1.110465	5.185475
13	1	0	0.948015	0.039887	1.874451

Zero-point correction= 0.078717 (Hartree/Particle)
Thermal correction to Energy= 0.090287
Thermal correction to Enthalpy= 0.091231
Thermal correction to Gibbs Free Energy= 0.037699
Sum of electronic and zero-point Energies= -1539.419656
Sum of electronic and thermal Energies= -1539.408087
Sum of electronic and thermal Enthalpies= -1539.407142
Sum of electronic and thermal Free Energies= -1539.460674

11. transition state for reaction 3 (TS3)

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.330738
3	6	0	0.907609	0.000000	-1.074948
4	6	0	0.709897	0.882678	-2.181233
5	50	0	-1.465765	0.218584	-1.817137
6	17	0	-2.153576	-2.031151	-1.689757
7	17	0	-2.754642	1.874804	-0.753124
8	17	0	-2.158918	0.617377	-4.070193
9	1	0	-0.924311	-0.121526	1.889401

10	1	0	0.899537	0.184591	1.918961
11	1	0	1.520252	-0.892977	-1.236412
12	1	0	1.244844	0.705384	-3.106880
13	1	0	0.529971	1.936968	-1.948704

	1	2	3
	?A	?A	?A
Frequencies --	-530.8666	36.4412	64.3383

Zero-point correction=	0.076149 (Hartree/Particle)
Thermal correction to Energy=	0.087323
Thermal correction to Enthalpy=	0.088268
Thermal correction to Gibbs Free Energy=	0.036467
Sum of electronic and zero-point Energies=	-1539.342317
Sum of electronic and thermal Energies=	-1539.331143
Sum of electronic and thermal Enthalpies=	-1539.330198
Sum of electronic and thermal Free Energies=	-1539.381999

12. molecular complex IN4a (PR1a + PR1a)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.073550	2.029590	-2.698084
2	6	0	-0.128753	2.196147	-1.418827
3	6	0	-0.340893	2.359595	-0.132400
4	6	0	0.526060	3.193209	0.764204
5	50	0	1.860356	1.940789	1.923376
6	17	0	3.551918	1.025334	0.563704
7	17	0	2.919962	3.055075	3.706289
8	17	0	0.708874	0.096805	2.836587
9	50	0	-2.032076	-1.803708	-1.161176
10	17	0	-2.595914	-1.305451	-3.391639
11	17	0	-2.846973	-3.973543	-0.744449
12	17	0	-3.294324	-0.333628	0.194503
13	6	0	0.100238	-1.672013	-0.805198
14	6	0	0.872505	-2.491516	-1.794225
15	6	0	1.505397	-1.986559	-2.827161
16	6	0	2.141271	-1.483681	-3.851239
17	1	0	-0.363719	2.701994	-3.433122

18	1	0	0.681680	1.209215	-3.075329
19	1	0	-1.197489	1.865777	0.326403
20	1	0	1.175303	3.876578	0.212652
21	1	0	-0.052709	3.758404	1.499335
22	1	0	0.898997	-3.569066	-1.634151
23	1	0	1.659372	-1.381256	-4.821432
24	1	0	3.178287	-1.163650	-3.773842
25	1	0	0.236762	-2.011459	0.224903
26	1	0	0.332998	-0.607263	-0.862812

Zero-point correction=	0.156547 (Hartree/Particle)
Thermal correction to Energy=	0.182382
Thermal correction to Enthalpy=	0.183326
Thermal correction to Gibbs Free Energy=	0.087227
Sum of electronic and zero-point Energies=	-3078.823991
Sum of electronic and thermal Energies=	-3078.798157
Sum of electronic and thermal Enthalpies=	-3078.797213
Sum of electronic and thermal Free Energies=	-3078.893312

13. transition state TS4

Z-Matrix orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.347626
3	6	0	1.174276	0.000000	2.138987
4	6	0	2.229758	-0.931892	2.020929
5	50	0	1.740463	-2.582633	3.713511
6	17	0	1.142351	-4.193624	5.352693
7	17	0	2.750514	-4.149327	2.229845
8	17	0	3.044038	-1.251179	5.202077
9	50	0	-1.928460	-0.031405	2.630349
10	17	0	-3.205050	-0.567459	0.668905
11	17	0	-3.890863	0.049013	4.044496
12	17	0	-1.141367	2.091787	3.498577
13	6	0	-1.051462	-1.862794	3.635518
14	6	0	-1.952597	-2.807612	4.327694
15	6	0	-2.368856	-3.941579	3.804268
16	-1	0	-2.185605	-3.339483	2.701177
17	6	0	-2.773011	-5.068081	3.288006

18	1	0	0.921075	0.145229	-0.566210
19	1	0	-0.924431	-0.055516	-0.565728
20	1	0	1.206714	0.693924	2.983202
21	1	0	2.268302	-1.536379	1.116873
22	1	0	3.182385	-0.671392	2.477423
23	1	0	-2.316116	-2.507829	5.308301
24	1	0	-3.654691	-5.115692	2.651944
25	1	0	-2.245936	-6.000537	3.481357
26	1	0	-0.365987	-1.331247	4.322598
27	1	0	-0.585082	-2.285818	2.727703

	1	2	3
	?A	?A	?A
Frequencies --	-291.4533	14.8417	18.1170

Zero-point correction=	0.155821 (Hartree/Particle)
Thermal correction to Energy=	0.179935
Thermal correction to Enthalpy=	0.180879
Thermal correction to Gibbs Free Energy=	0.095321
Sum of electronic and zero-point Energies=	-3078.722872
Sum of electronic and thermal Energies=	-3078.698758
Sum of electronic and thermal Enthalpies=	-3078.697814
Sum of electronic and thermal Free Energies=	-3078.783373

14. molecular complex IN4b (PR1a + PR2)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.359028	0.714852	-3.076073
2	6	0	0.255764	1.714049	-2.188663
3	6	0	1.366259	2.539336	-1.685956
4	6	0	2.550925	2.036950	-1.315229
5	50	0	1.773589	-1.942059	1.617656
6	17	0	2.714093	-3.954071	2.401572
7	17	0	1.827556	-2.076259	-0.739995
8	17	0	3.279534	-0.219101	2.201041
9	50	0	-1.678988	2.120192	-1.404374
10	17	0	-3.320406	0.775819	-2.420524
11	17	0	-1.844480	1.739288	0.920375
12	17	0	-2.323179	4.360151	-1.696419

13	6	0	-0.240563	-1.660063	2.365430
14	6	0	-1.135864	-2.783014	1.934684
15	6	0	-2.002447	-2.688386	0.952732
16	6	0	-2.868325	-2.589803	-0.018583
17	1	0	1.321382	0.491288	-3.532803
18	1	0	-0.482554	0.101350	-3.383224
19	1	0	1.188060	3.611436	-1.606205
20	1	0	2.749231	0.969405	-1.332447
21	1	0	3.350114	2.685110	-0.970134
22	1	0	-1.046966	-3.725058	2.475110
23	1	0	-3.884066	-2.243330	0.158273
24	1	0	-2.604397	-2.846972	-1.042070
25	1	0	-0.127836	-1.603352	3.451538
26	1	0	-0.564685	-0.689122	1.984970

Zero-point correction=	0.157108 (Hartree/Particle)
Thermal correction to Energy=	0.182904
Thermal correction to Enthalpy=	0.183848
Thermal correction to Gibbs Free Energy=	0.089142
Sum of electronic and zero-point Energies=	-3078.833794
Sum of electronic and thermal Energies=	-3078.807998
Sum of electronic and thermal Enthalpies=	-3078.807053
Sum of electronic and thermal Free Energies=	-3078.901759

15. molecular complex IN5a (PR1a + PR2)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.794144	4.431298	-0.302781
2	6	0	1.838465	3.650170	-0.333416
3	6	0	2.885588	2.858575	-0.371421
4	6	0	2.873099	1.499081	-1.003570
5	50	0	2.763501	-0.045155	0.513254
6	17	0	0.851302	0.154523	1.880301
7	17	0	2.756973	-2.263716	-0.304623
8	17	0	4.608468	0.100085	1.974956
9	50	0	-2.490861	-0.182539	-0.734713
10	17	0	-0.508126	-0.165572	-2.021099
11	17	0	-4.242003	-0.250813	-2.302911
12	17	0	-2.693624	1.917049	0.303327
13	6	0	-1.531438	-2.718641	0.531042

14	6	0	-2.512618	-1.811956	0.632505
15	6	0	-3.623779	-1.849971	1.597224
16	6	0	-4.337106	-2.950680	1.864677
17	1	0	0.590413	5.140215	-1.102364
18	1	0	0.084853	4.394135	0.521073
19	1	0	3.818636	3.186461	0.085966
20	1	0	2.005896	1.337247	-1.645838
21	1	0	3.789087	1.280247	-1.559048
22	1	0	-1.483026	-3.545591	1.237427
23	1	0	-0.743021	-2.669016	-0.213831
24	1	0	-3.869196	-0.916122	2.102464
25	1	0	-5.130446	-2.938681	2.605214
26	1	0	-4.154193	-3.887854	1.347129

Zero-point correction= 0.157024 (Hartree/Particle)
Thermal correction to Energy= 0.182852
Thermal correction to Enthalpy= 0.183796
Thermal correction to Gibbs Free Energy= 0.088679
Sum of electronic and zero-point Energies= -3078.833989
Sum of electronic and thermal Energies= -3078.808161
Sum of electronic and thermal Enthalpies= -3078.807216
Sum of electronic and thermal Free Energies= -3078.902334

16. transition state for reaction 5 (TS5)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.327187	1.029582	-3.334236
2	6	0	1.342565	1.054594	-2.015249
3	6	0	2.087636	1.064502	-0.855087
4	6	0	2.620194	-0.103360	-0.255296
5	50	0	1.088054	-1.103673	1.251403
6	17	0	-0.480762	-2.206831	2.671819
7	17	0	2.674075	-2.898893	1.319998
8	17	0	1.420121	0.773765	2.703428
9	50	0	-0.905680	1.195546	-1.020133
10	17	0	-2.222398	0.926770	-2.972708
11	17	0	-2.338695	1.396859	0.867510
12	17	0	-0.385241	3.551065	-1.014397
13	6	0	0.028646	-1.923425	-1.505761

14	6	0	-0.678692	-1.198722	-0.601890
15	6	0	-2.010729	-1.649924	-0.148241
16	6	0	-2.916352	-2.159971	-0.995386
17	1	0	2.259270	1.158144	-3.883514
18	1	0	0.416589	0.934401	-3.917768
19	1	0	2.121341	1.998760	-0.290350
20	1	0	2.826759	-0.947465	-0.910384
21	1	0	3.380360	0.072277	0.504218
22	1	0	-0.325706	-2.904832	-1.820315
23	1	0	0.947835	-1.572245	-1.962324
24	1	0	-2.267049	-1.511292	0.893923
25	1	0	-3.887339	-2.482317	-0.633584
26	1	0	-2.734232	-2.245239	-2.062613

	1	2	3
	?A	?A	?A
Frequencies --	-243.6514	23.7975	28.9981

Zero-point correction= 0.157531 (Hartree/Particle)
Thermal correction to Energy= 0.181396
Thermal correction to Enthalpy= 0.182340
Thermal correction to Gibbs Free Energy= 0.100576
Sum of electronic and zero-point Energies= -3078.752643
Sum of electronic and thermal Energies= -3078.728778
Sum of electronic and thermal Enthalpies= -3078.727834
Sum of electronic and thermal Free Energies= -3078.809598

17. molecular complex IN5b (PR2 + PR2)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.361111	1.131838	-4.473442
2	6	0	-0.393598	0.986019	-3.141298
3	6	0	0.766145	1.066165	-2.238543
4	6	0	1.936878	0.462831	-2.481543
5	50	0	2.272522	-0.671258	2.235458
6	17	0	3.478984	-0.821336	4.246050
7	17	0	3.051387	-2.370631	0.808701
8	17	0	2.951524	1.365049	1.255265
9	50	0	-2.290300	0.574994	-2.264827

10	17	0	-4.023653	0.828510	-3.829495
11	17	0	-2.493951	-1.607599	-1.399650
12	17	0	-2.760432	1.994581	-0.445655
13	6	0	-0.501781	-1.704983	1.813708
14	6	0	0.172213	-0.805730	2.544763
15	6	0	-0.413255	0.113727	3.534437
16	6	0	-1.528156	0.822691	3.318332
17	1	0	0.575315	1.382763	-4.968914
18	1	0	-1.237537	1.028690	-5.106406
19	1	0	0.644919	1.646644	-1.324376
20	1	0	2.084630	-0.163089	-3.357027
21	1	0	2.773342	0.574974	-1.799534
22	1	0	-1.571699	-1.836781	1.963642
23	1	0	-0.034639	-2.337350	1.064822
24	1	0	0.114275	0.217115	4.482415
25	1	0	-1.935962	1.470017	4.088394
26	1	0	-2.053342	0.789085	2.368252

Zero-point correction= 0.157822 (Hartree/Particle)
Thermal correction to Energy= 0.183448
Thermal correction to Enthalpy= 0.184392
Thermal correction to Gibbs Free Energy= 0.089921
Sum of electronic and zero-point Energies= -3078.842808
Sum of electronic and thermal Energies= -3078.817182
Sum of electronic and thermal Enthalpies= -3078.816238
Sum of electronic and thermal Free Energies= -3078.910709

18. molecular complex IN6a (PR1a + PR1a)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	-2.924949	1.090850	0.336313
2	6	0	-2.823089	1.240889	2.495817
3	6	0	-1.419854	1.123719	3.009955
4	6	0	-0.936394	0.043603	3.577347
5	6	0	-0.456814	-1.031495	4.141282
6	17	0	-2.095620	-0.975634	-0.434330
7	17	0	-5.155570	1.231796	-0.423204
8	17	0	-1.732540	2.794465	-0.753855
9	50	0	2.979787	-0.595950	-0.809432

10	6	0	2.966085	-2.680696	-0.219838
11	6	0	1.654427	-3.342989	-0.518630
12	6	0	0.754702	-3.641780	0.388607
13	6	0	-0.146164	-3.947519	1.283143
14	17	0	5.168852	0.286058	-0.832518
15	17	0	1.739151	0.742238	0.678402
16	17	0	2.096346	-0.280423	-2.962705
17	1	0	-0.532125	-1.194064	5.214444
18	1	0	0.042039	-1.800552	3.554884
19	1	0	-0.772705	1.991874	2.890042
20	1	0	-3.474759	0.446489	2.866437
21	1	0	-3.275769	2.209346	2.726699
22	1	0	3.205355	-2.681004	0.845765
23	1	0	3.796817	-3.129449	-0.771909
24	1	0	1.446993	-3.580810	-1.561557
25	1	0	-0.948317	-3.255580	1.530650
26	1	0	-0.137387	-4.908148	1.794008

Zero-point correction= 0.156334 (Hartree/Particle)
Thermal correction to Energy= 0.182285
Thermal correction to Enthalpy= 0.183229
Thermal correction to Gibbs Free Energy= 0.086412
Sum of electronic and zero-point Energies= -3078.820733
Sum of electronic and thermal Energies= -3078.794781
Sum of electronic and thermal Enthalpies= -3078.793837
Sum of electronic and thermal Free Energies= -3078.890655

19. transition state for reaction 6 (TS)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	-1.884466	0.934279	-1.150058
2	6	0	-1.926538	1.159338	1.108297
3	6	0	-0.617834	0.911504	1.681186
4	6	0	-0.182357	-0.305478	2.134284
5	6	0	-0.420927	-1.245529	3.047909
6	17	0	-1.547171	0.219874	-3.431509
7	17	0	-4.221540	1.355534	-1.306884
8	17	0	-0.408322	2.802422	-1.343232
9	50	0	1.972379	-0.840775	1.073340

10	6	0	0.789918	-2.377458	-0.106898
11	6	0	-0.149280	-1.733873	-1.004703
12	6	0	-1.452190	-1.445646	-0.695720
13	6	0	-2.616461	-2.009127	-0.375826
14	17	0	3.116842	-2.544043	2.278982
15	17	0	2.718105	1.029614	2.405563
16	17	0	2.985432	-0.028750	-0.931739
17	1	0	-0.996351	-1.011748	3.943381
18	1	0	0.017140	-2.239564	3.008746
19	1	0	0.112408	1.720934	1.631142
20	1	0	-2.701484	0.471709	1.449585
21	1	0	-2.224137	2.206565	1.181280
22	1	0	0.324342	-3.018208	0.643111
23	1	0	1.607524	-2.867824	-0.637629
24	1	0	0.244782	-1.339476	-1.942828
25	1	0	-3.460718	-1.449993	0.019313
26	1	0	-2.802021	-3.059043	-0.601401

	1	2	3
	?A	?A	?A
Frequencies --	-428.9893	13.9008	24.8390

Zero-point correction= 0.156942 (Hartree/Particle)
Thermal correction to Energy= 0.180737
Thermal correction to Enthalpy= 0.181682
Thermal correction to Gibbs Free Energy= 0.098925
Sum of electronic and zero-point Energies= -3078.749115
Sum of electronic and thermal Energies= -3078.725319
Sum of electronic and thermal Enthalpies= -3078.724375
Sum of electronic and thermal Free Energies= -3078.807131

20. molecular complex IN6b (PR2 + PR2)

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	50	0	-2.169996	0.694473	-2.560965
2	6	0	-1.615148	1.027214	1.923496
3	6	0	-0.439538	0.877397	2.546774
4	6	0	0.219612	-0.423076	2.745512

5	6	0	-0.393580	-1.559581	3.108218
6	17	0	-2.058785	0.800426	-4.904682
7	17	0	-4.366679	1.250861	-1.924422
8	17	0	-0.780662	2.416196	-1.779128
9	50	0	2.330246	-0.511540	2.461257
10	6	0	0.396683	-2.418290	-1.165225
11	6	0	-0.320137	-1.744511	-2.073617
12	6	0	-1.684853	-1.249447	-1.833494
13	6	0	-2.659863	-1.925797	-1.208098
14	17	0	3.071253	-2.729541	2.728771
15	17	0	3.476102	0.815999	4.023719
16	17	0	3.073146	0.202039	0.353003
17	1	0	-1.458060	-1.555519	3.337040
18	1	0	0.125865	-2.507979	3.209334
19	1	0	0.080086	1.758406	2.921965
20	1	0	-2.141264	0.180435	1.491620
21	1	0	-2.074999	2.004147	1.817208
22	1	0	0.012600	-2.610795	-0.167342
23	1	0	1.392919	-2.782914	-1.392646
24	1	0	0.120931	-1.528736	-3.046167
25	1	0	-3.644796	-1.508725	-1.019783
26	1	0	-2.489193	-2.950086	-0.880690

Zero-point correction= 0.157762 (Hartree/Particle)
Thermal correction to Energy= 0.183428
Thermal correction to Enthalpy= 0.184373
Thermal correction to Gibbs Free Energy= 0.087254
Sum of electronic and zero-point Energies= -3078.839446
Sum of electronic and thermal Energies= -3078.813780
Sum of electronic and thermal Enthalpies= -3078.812835
Sum of electronic and thermal Free Energies= -3078.909954