Electronic Supplementary Material (ESI) for Dalton Transactions

Mechanistic Study on the Palladium-Catalyzed (3 + 2) Intramolecular Cycloaddition of Alk-5-enylidenecyclopropanes

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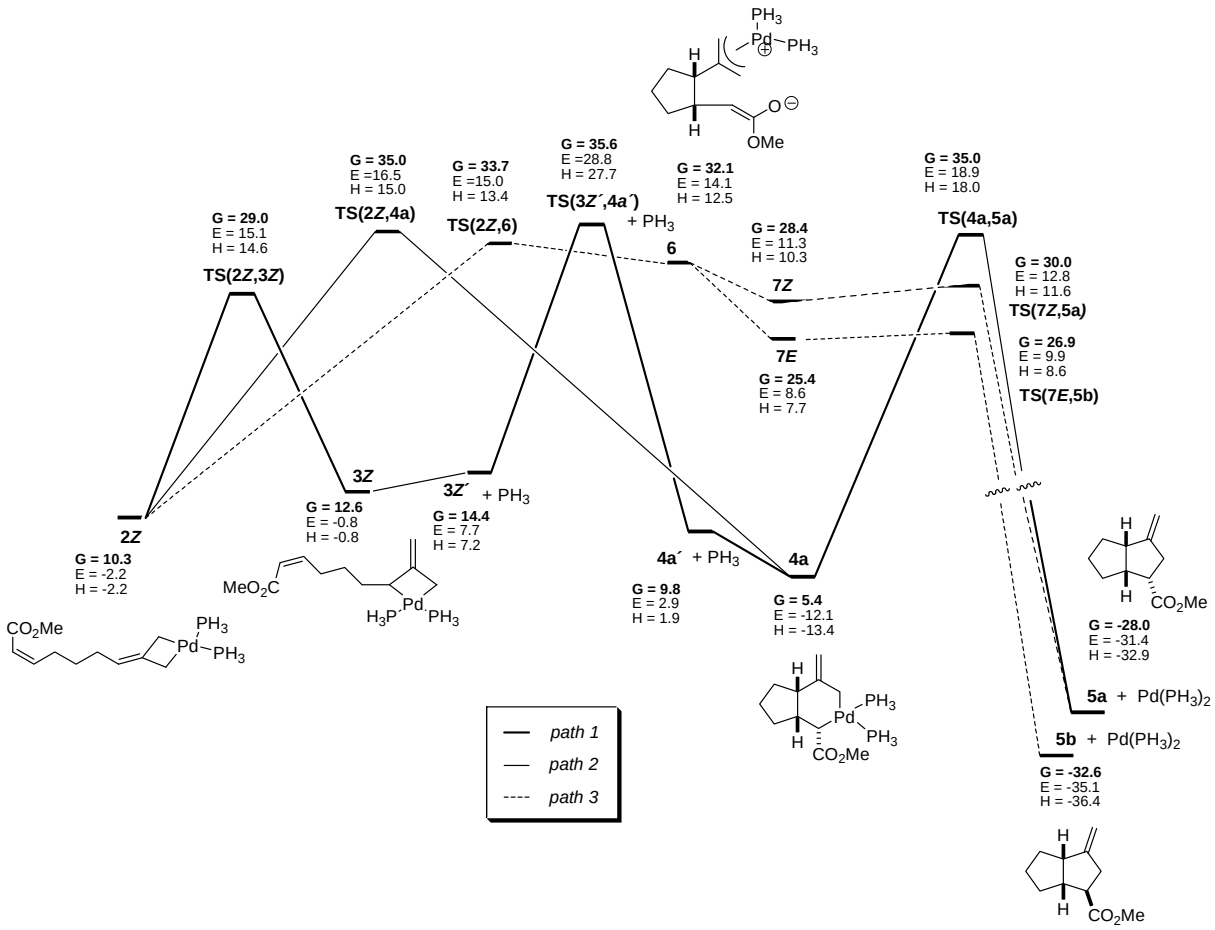
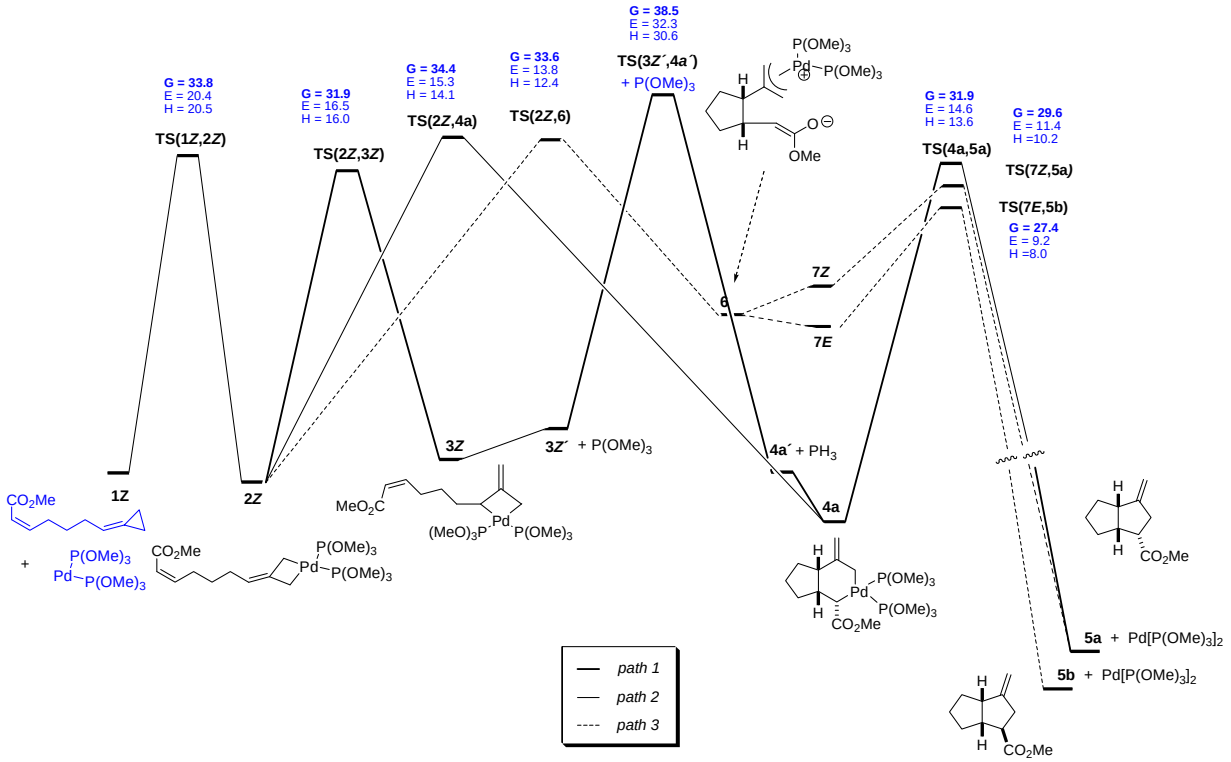
1. Additional Schemes on calculations

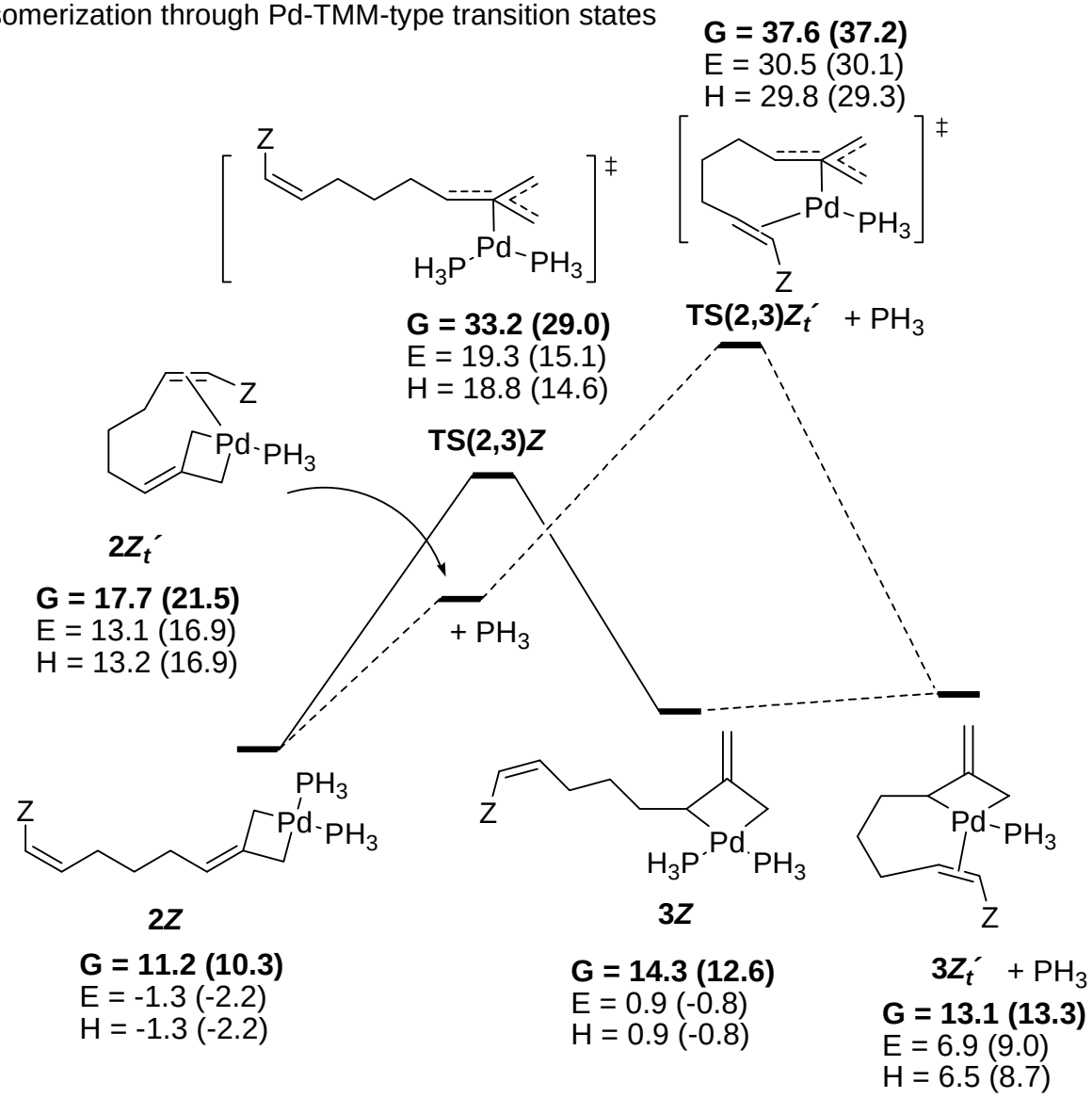


Scheme S1. **Gas-phase** electronic energy, enthalpy, and Gibbs free energy (bold) calculated for *cis*-fused products involved in *paths 1*, *2* and *3* for precursor **1*Z*** and considering the coordination of two PH_3 ligands to the Pd. All values are referred to systems **1*Z*** + $Pd(PH_3)_2$**. (Stationary points are the same as included in the Scheme 7 of the main text)**

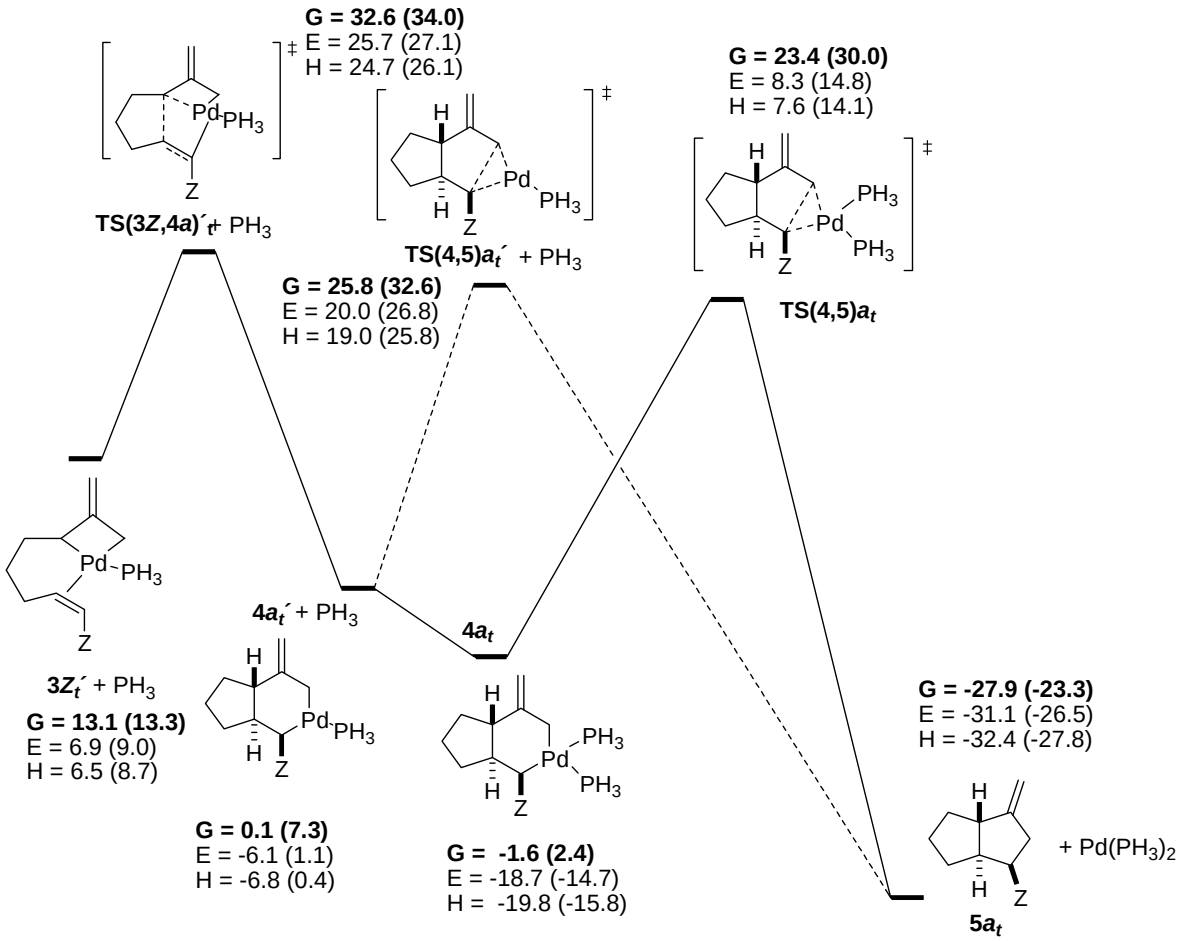


Scheme S2. Electronic energy, enthalpy, and Gibbs free energy (bold) calculated for cis-fused products involved in paths 1, 2 and 3 for precursor 1Z and considering the coordination of two $P(OMe)_3$ ligands to the Pd. All values are referred to systems 1Z + $Pd[P(OMe)_3]_2$. Only starting compounds and transition states have been calculated. Calculated stationary points have been **fully optimized in acetonitrile using the PCM model**.

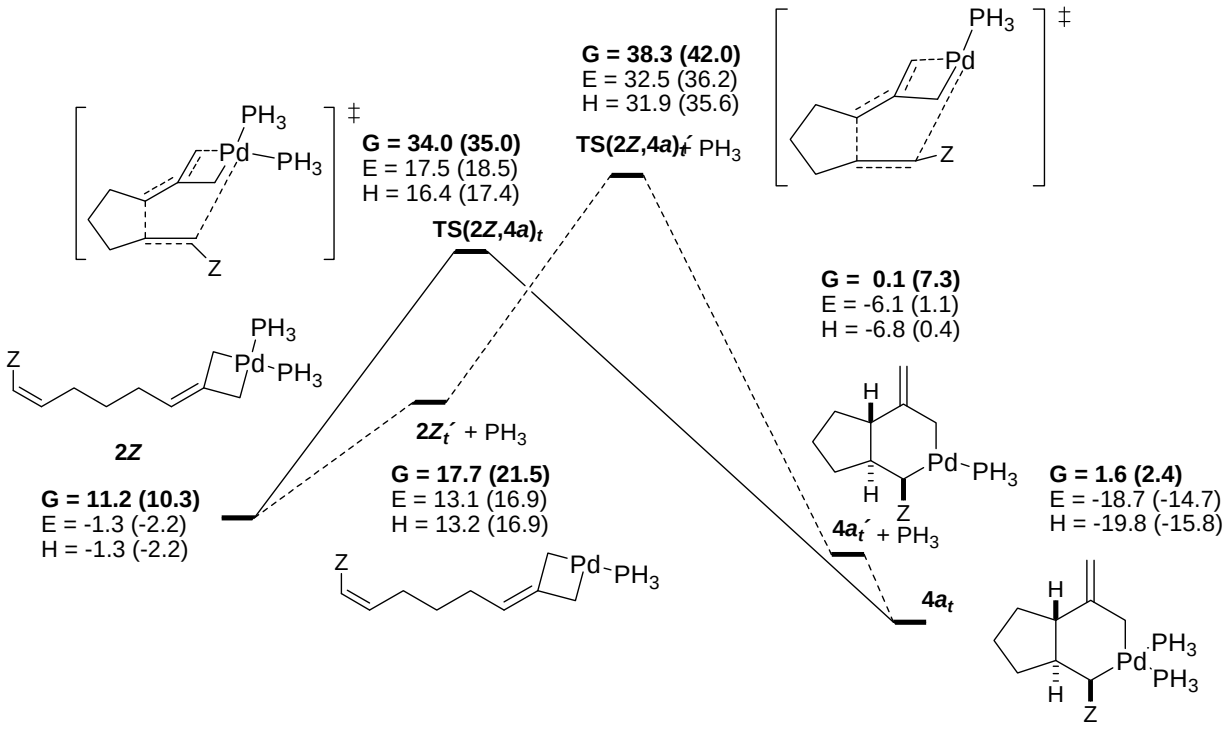
a) Isomerization through Pd-TMM-type transition states



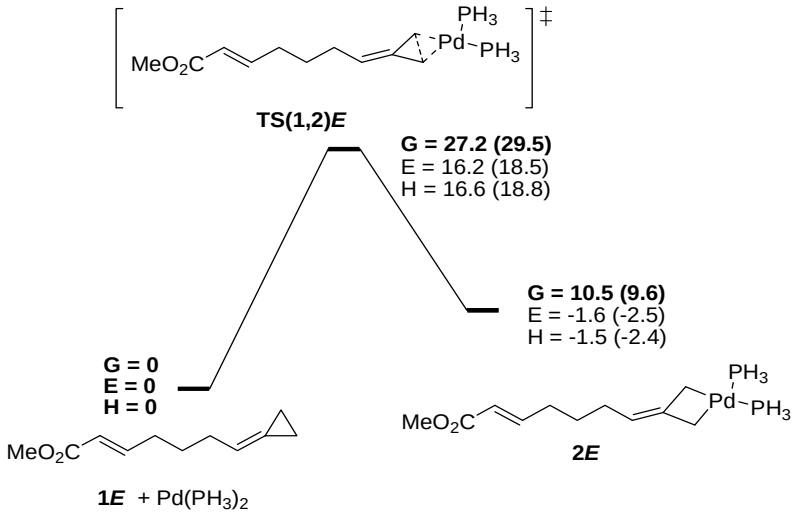
b) Carbometallation reaction and C-C reductive elimination



Scheme S3. Electronic energy, enthalpy, and Gibbs free energy (bold) calculated for intermediates involved in *path 1* for system **1*Z***, leading to a *trans* fusion between the rings formed. All values are given in kcal mol^{-1} and referred to systems **1*Z***+$Pd(PH_3)_2$, respectively. Dashed lines connect complexes with only one PH_3 ligand.

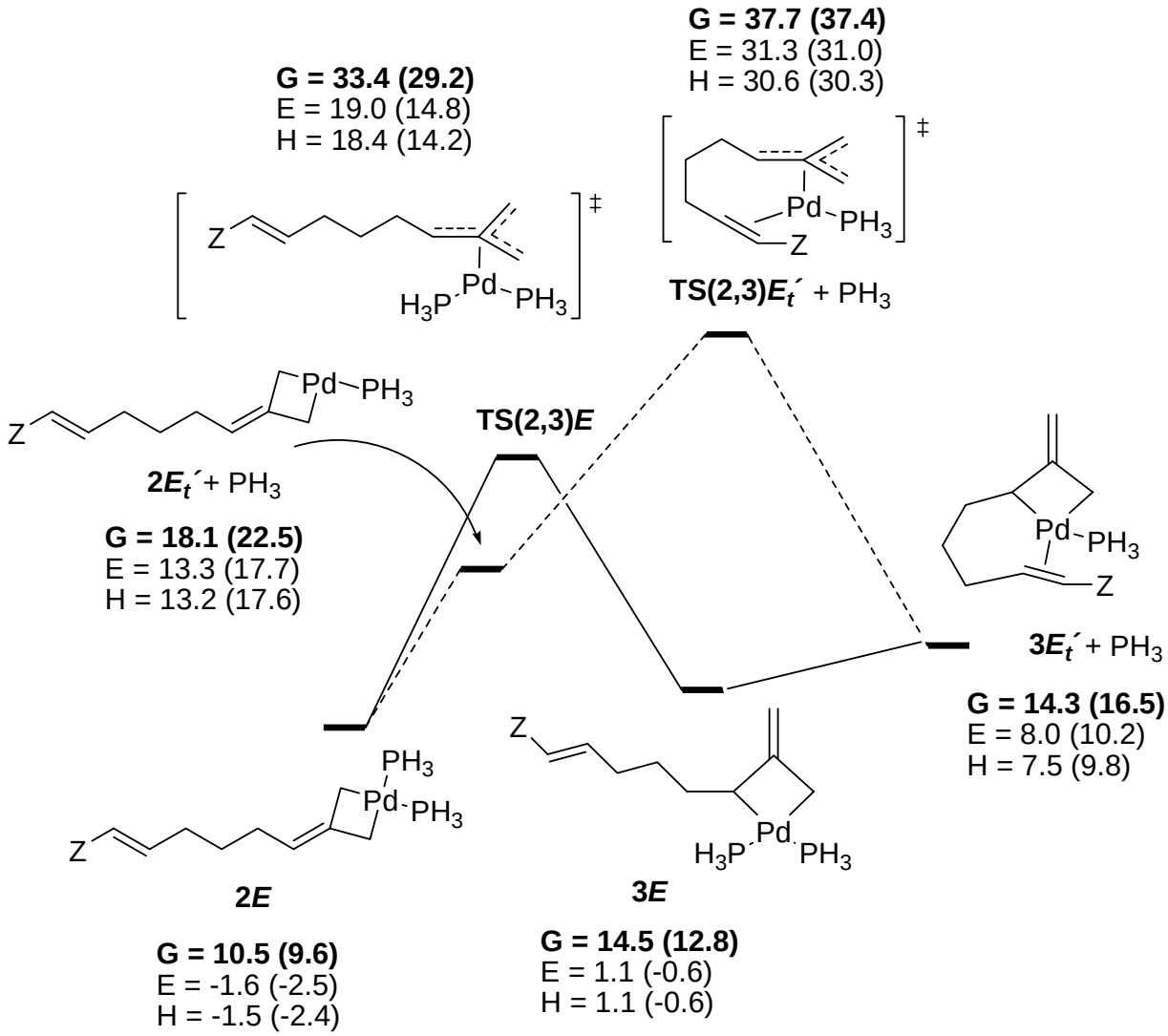


Scheme S4. Electronic energy, enthalpy, and Gibbs free energy (bold) calculated for intermediates involved in *path 2* for system **1*Z*** leading to *trans* fusion between the rings formed. All values are given in kcal mol^{-1} and referred to systems **1*Z*** + $Pd(PH_3)_2$. Dashed lines connect complexes with only one PH_3 ligand.

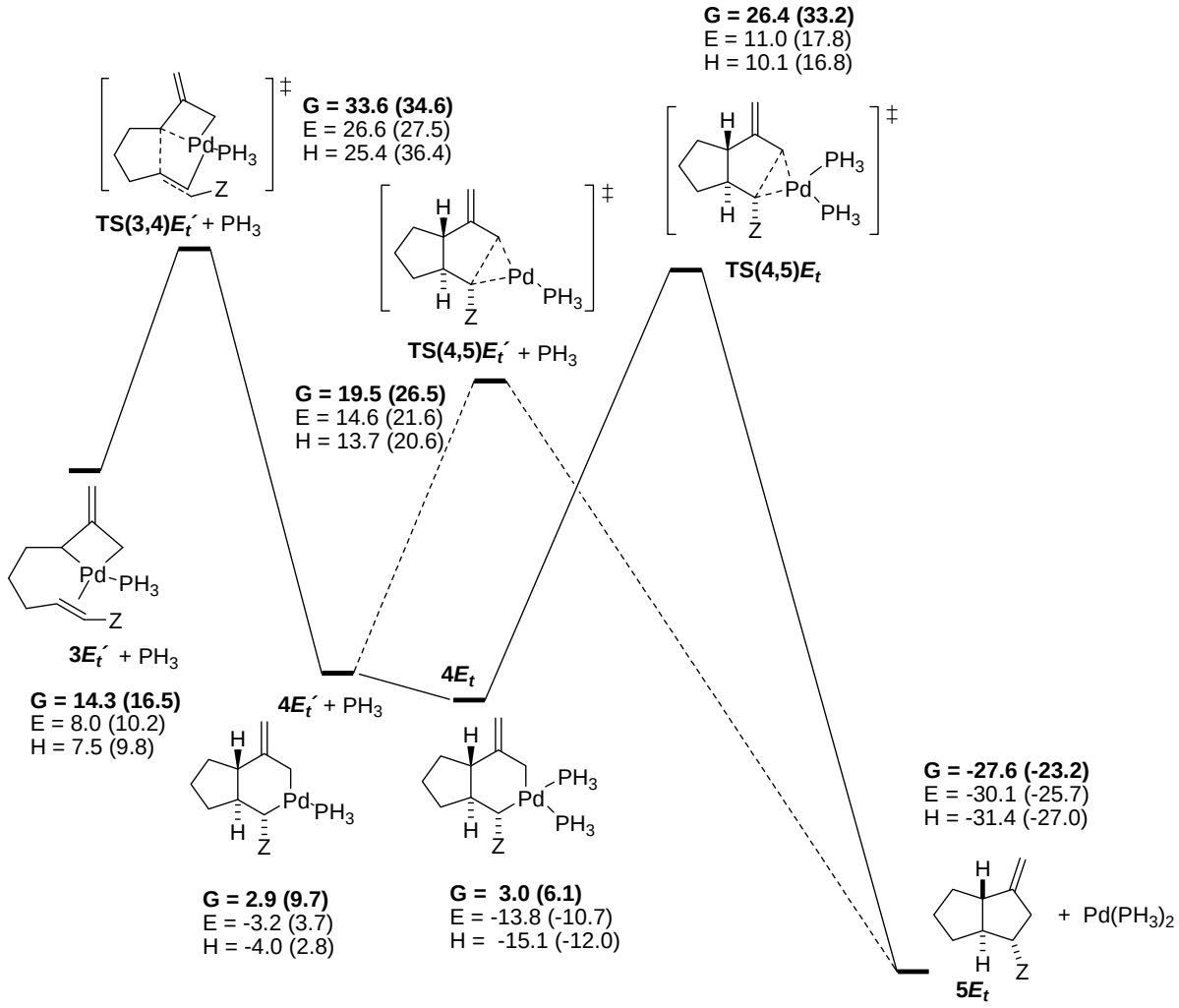


Scheme S5. Electronic energy, enthalpy, and Gibbs free energy (bold) calculated for intermediates involved in the initial C-C oxidative addition step.

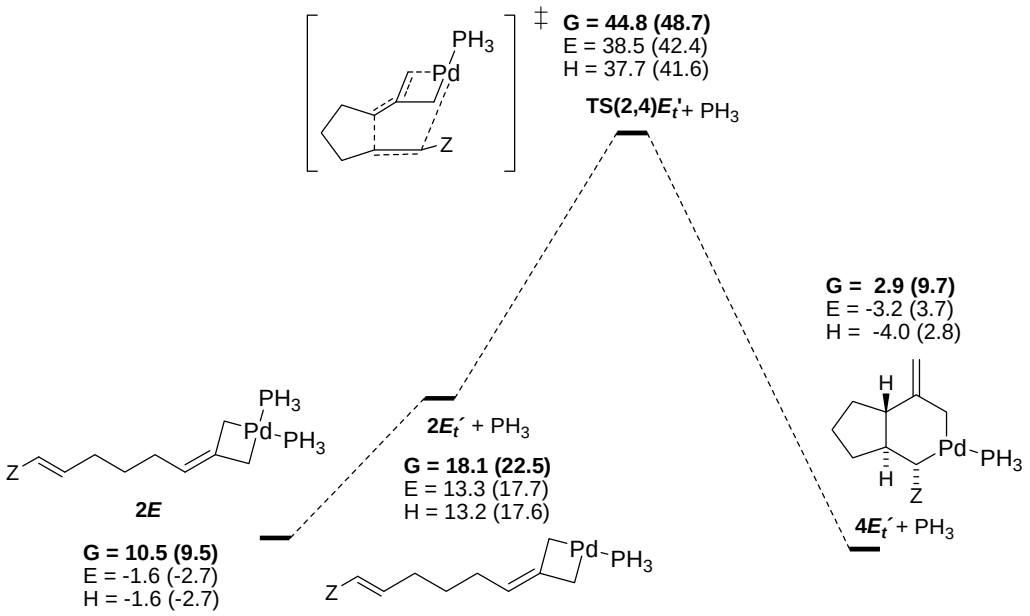
a) Isomerization through Pd-TMM-type transition states



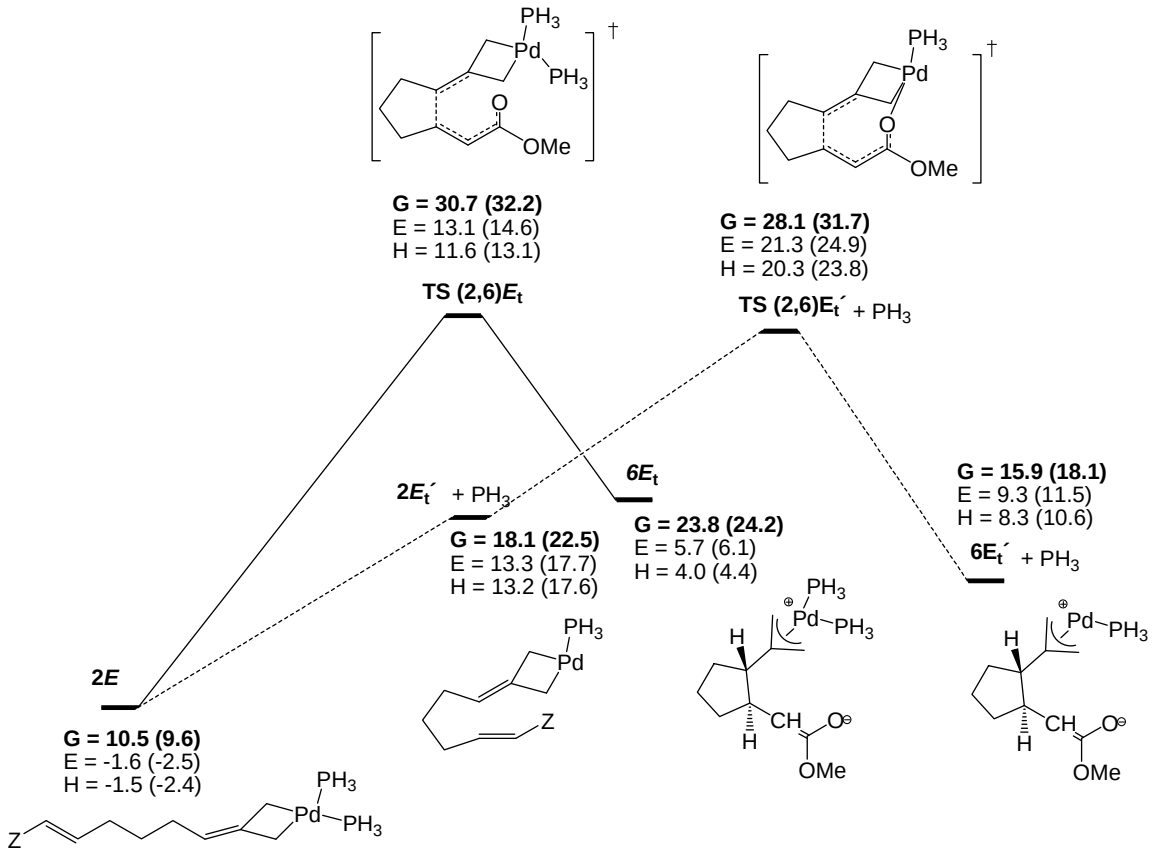
b) Carbometallation reaction and C-C reductive elimination



Scheme S6. Electronic energy, enthalpy, and Gibbs free energy (bold) calculated for intermediates involved in *path 1* for system **1*E***, leading to a *trans* fusion between the rings formed. All values are referred to **1*E***+$Pd(PH_3)_2$. Dashed lines connect complexes with only one PH_3 ligand.



Scheme S7. Electronic energy, enthalpy, and Gibbs free energy (bold) calculated for intermediates involved in *path 2* for system **1*E*** leading to a *trans* fusion (only the transition state with one phosphane was found). All values referred to systems **1*E*** + $Pd(PH_3)_2$. Dashed lines connect complexes with only one PH_3 ligand.

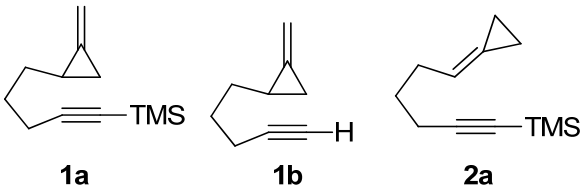


Scheme S8. Electronic energy, enthalpy, and Gibbs free energy (bold) calculated for intermediates involved in *path 3* for system **1*E*** leading to a *trans* fusion. All values referred to systems **1*E*** + $Pd(PH_3)_2$. Dashed lines connect complexes with only one PH_3 ligand.

2. Additional experimental results

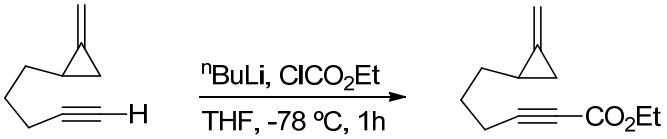
SYNTHESIS OF SUBSTRATES FOR CYCLOADDITION.

Trimethyl(5-(2-methylenecyclopropyl)pent-1-yn-1-yl)silane **(1a)**, 1-methylene-2-(pent-4-yn-1-yl)cyclopropane **(1b)**, (6-cyclopropylidenehex-1-yn-1-yl)trimethylsilane **(2a)** were prepared according to a method reported by de Mejiere et. al.[1]



1a **1b** **2a**

Ethyl 6-(2-methylenecyclopropyl)hex-2-ynoate (2)



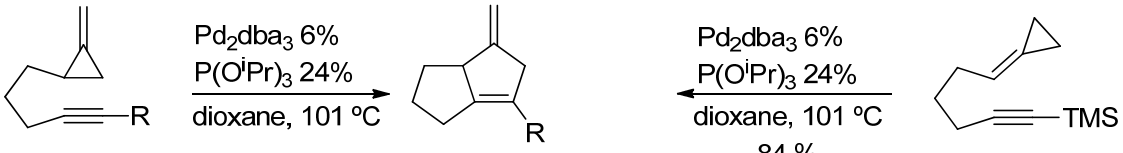
1a **1c**

To a solution of **1a** (120 mg, 1.0 mmol) in THF (2 mL) cooled at -78 ºC were added 0.56 mL of ^{n}BuLi (1.4 mmol, 2.5 M in hexanos). The mixture was stirred for 30 min and ethyl chloroformiate (0.20 mL, 2.0 mmol). The resulting solution was stirred for 1h at -78 ºC and then warmed up to room temperatura. The solution was poured into water (20 mL) and extracted with Et_2O (2x20 mL). The combined organic phases were dried over anhydrous Na_2SO_4, filtered and concentrated to afford a crude oil that was purified by chromatography in silica (100 % pentane) to give 78 mg of ester **1c** (41 %, colorless oil). **^{1}H-RMN** δ (ppm): 5.38 (1H, m), 5.33 (1H, m), 4.18 (2H, c, *J* = 7.1 Hz), 2.37 (1H, m), 1.75-1.16 (8H, m), 0.92 (2H, t, *J* = 0.92 Hz), 0.73 (1H, m); **^{13}C-RMN** δ (ppm): 153.7 (CO), 136.1 (C), 102.9 (CH_2), 89.0 (C), 73.3 (C), 61.7 (CH_2), 32.0 (CH_2), 27.3 (CH_2), 18.3 (CH_2), 14.9 (CH), 14.0 (CH_3), 9.3 (CH_2). **EMBR** (*m/z*, *I*): 193 ([M^+ +1], 33), 119 (100); **EMAR** calculated for $C_{12}H_{17}O_2$ 193.1229, found 193.1221.

General procedure for cycloaddition [ejemplificated for compound 2a]

To a solution of **2a** (50 mg, 0.26 mmol) in dioxane (5.2 mL) was added $P(O^{i}Pr)_3$ (16.0 μL, 24%) and Pd_2dba_3 (14.6 mg, 6%). The resulting mixture was stirred at 101 ºC for 3h. Then the resulting mixture was diluted with hexanes (5 mL) and filtered throgh a pad of silica eluting with Et_2O. The fíltrate was concentrated and purified by chromatography on silica (100% hexanes) to afford cycloadduct **3a** (colorless oil, 42 mg, 84 %).

[1] de Meijere, A.; Becker, H.; Stolle, A.; Kozhushkov, S. I.; Bes, M. T.; Salaün J.; Noltemeyer, M. *Chem. Eur. J.* **2005**, *11*, 2471.

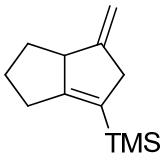


1a, R=TMS
1c, R=CO_2Et

3a, R = TMS, 70%
3c, R = CO_2Et, 77 %

2a

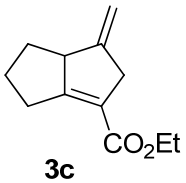
Trimethyl(3-methylene-2,3,3a,4,5,6-hexahydropentalen-1-yl)silane (3a).



3a

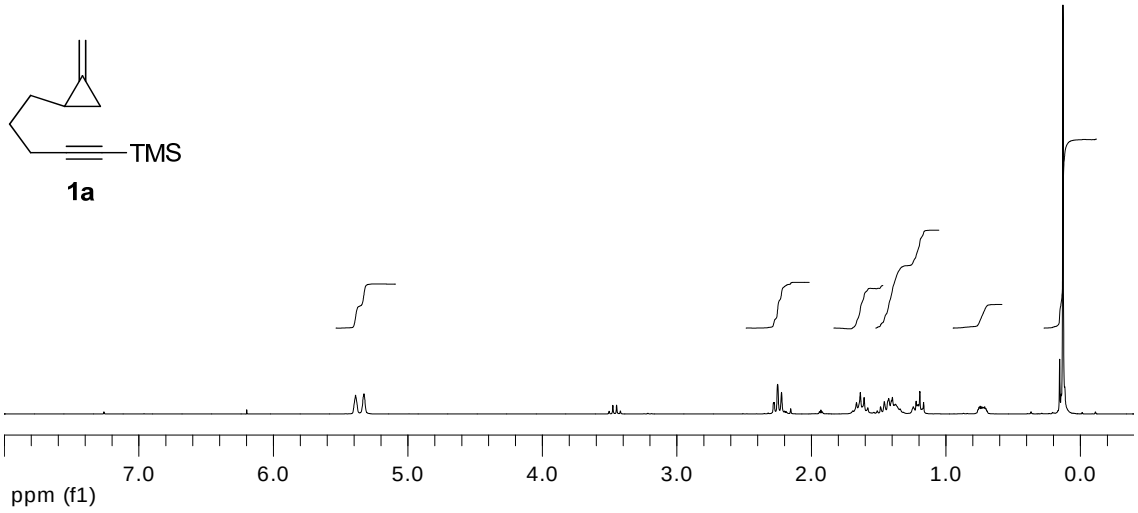
Colorless oil. **^{1}H-RMN** δ (ppm): 4.80(1H, ddt, *J* = 3.8, 2.5 y 1.3 Hz), 4.75 (1H, ddd, *J* = 4.0, 2.8 y 1.4 Hz), 3.52-3.38 (2H, m), 3.15 (1H, m), 2.26-2.16 (2H, m), 2.05-1.89 (3H, m), 1.27-1.09 (2H, m), 0.08 (9H, s); **^{13}C-RMN** δ (ppm): 163.3 (C), 155.3 (C), 128.1 (C), 104.3 (CH_2), 57.8 (CH), 48.1(CH_2), 28.7 (CH_2), 28.5 (CH_2), 25.3 (CH_2), -1.1 (CH_3).

ethyl 3-methylene-2,3,3a,4,5,6-hexahydropentalene-1-carboxylate (3c).



3c

Colorless oil [77 %]. **^{1}H-RMN** δ (ppm): 4.88 (1H, m), 4.82 (1H, m), 4.17 (2H, c, *J* = 7.1), 3.65-3.55 (2H, m), 3.40 (1H, ddt, *J* = 19.2, 3.4 y 1.7 Hz), 2.63 (1H, m), 2.43 (1H, m), 2.11-1.98 (3H, m), 1.28 (3H, t, *J* = 7.1 Hz), 0.90 (1H, m); **^{13}C-RMN** δ (ppm): 168.7 (C), 151.1 (C), 121.6 (C), 106.8 (CH_2), 59.8 (CH_2), 58.0(CH), 43.4 (CH_2), 28.7 (CH_2), 28.0 (CH_2), 26.1 (CH_2), 14.4 (CH_3).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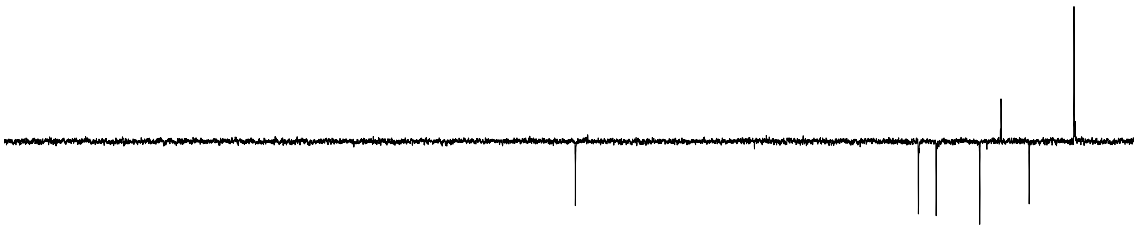
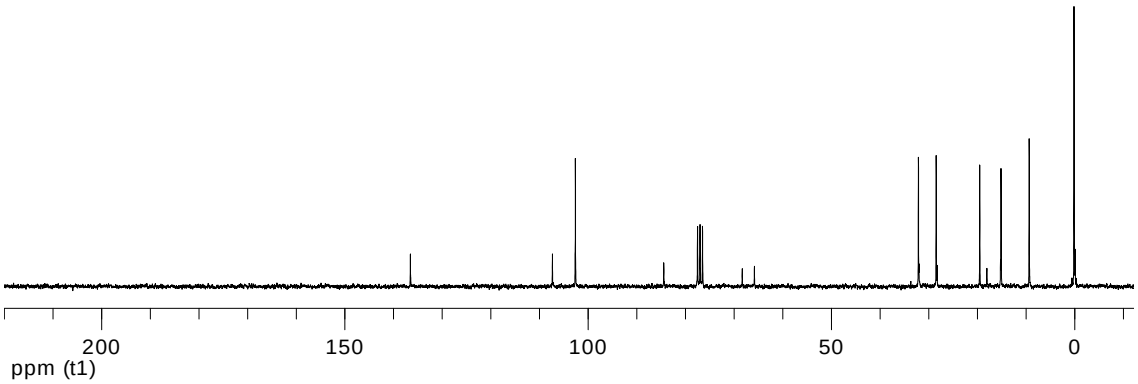
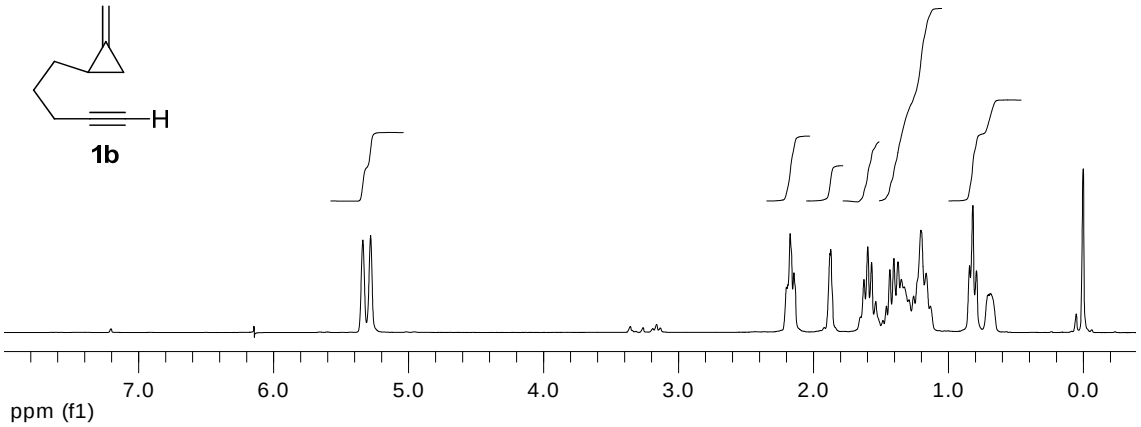
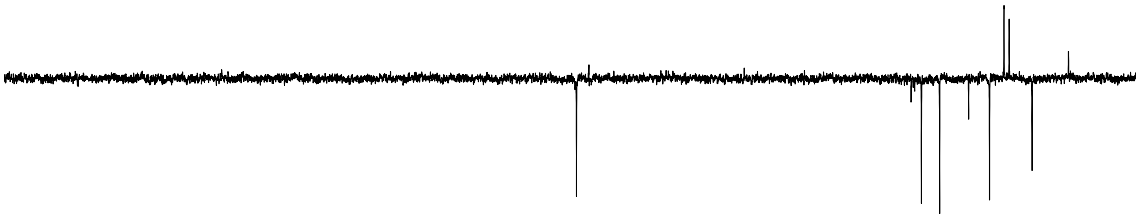
1a
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)

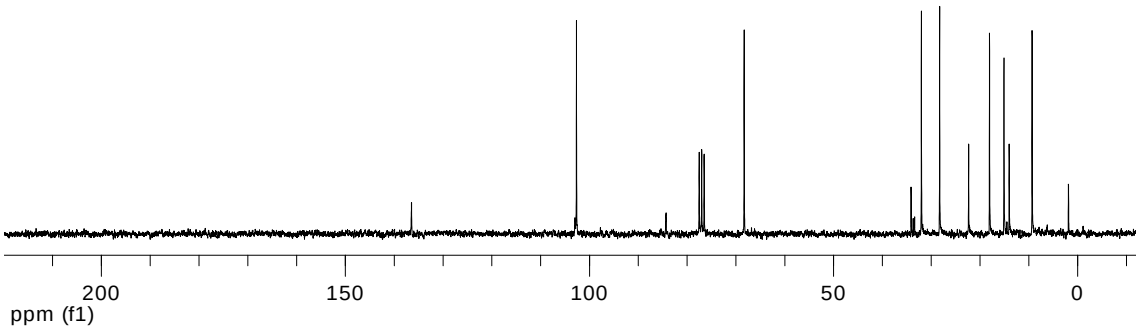


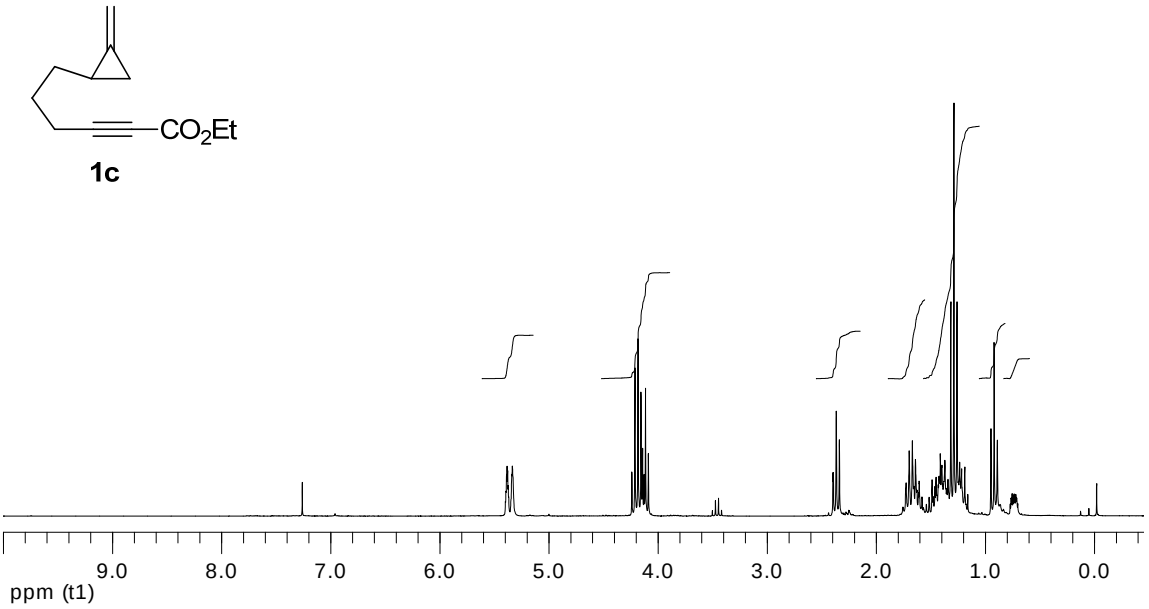

200
150
100
50
0
ppm (t1)



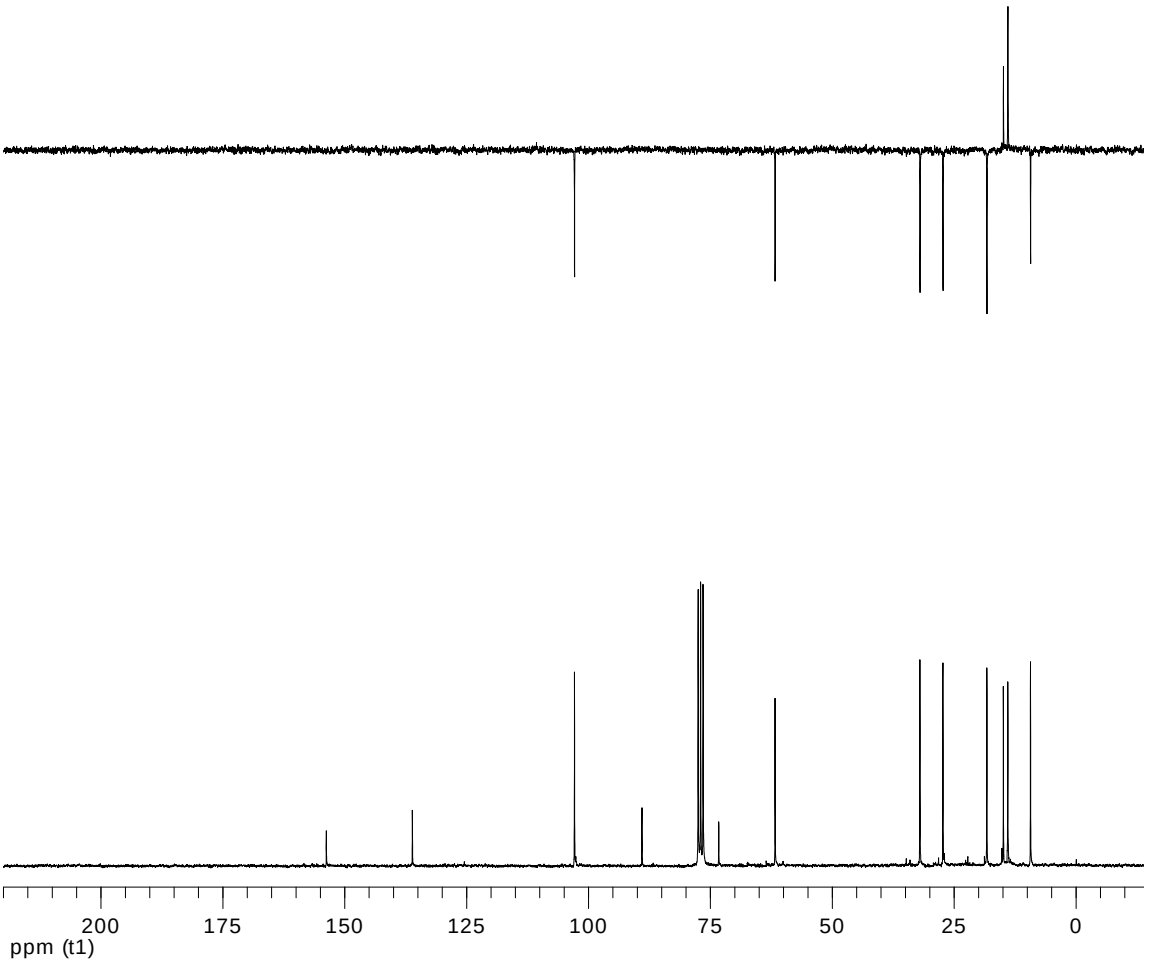
1b

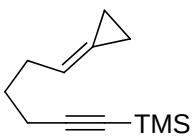




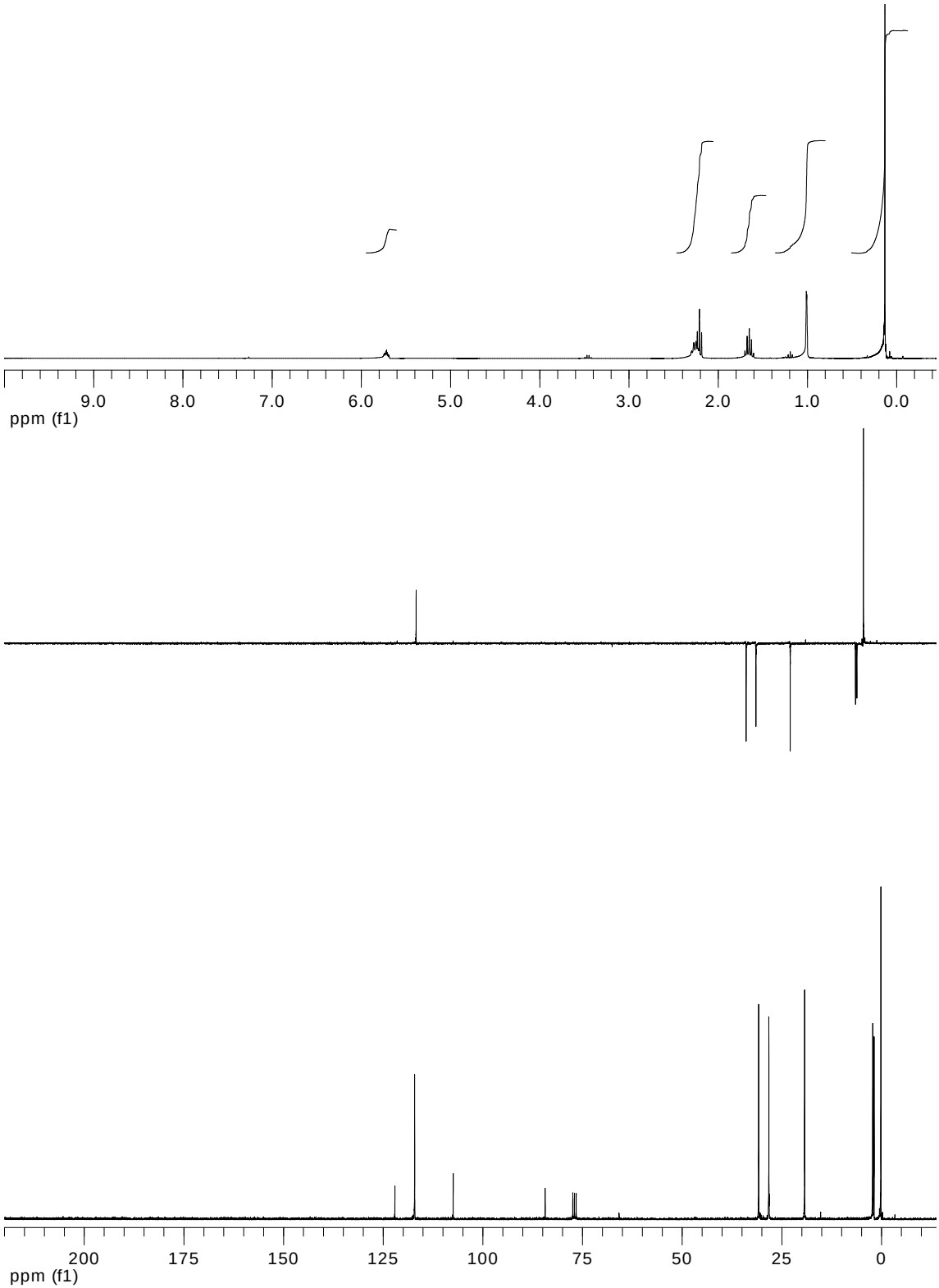


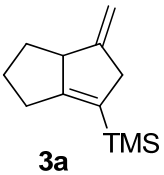
1c



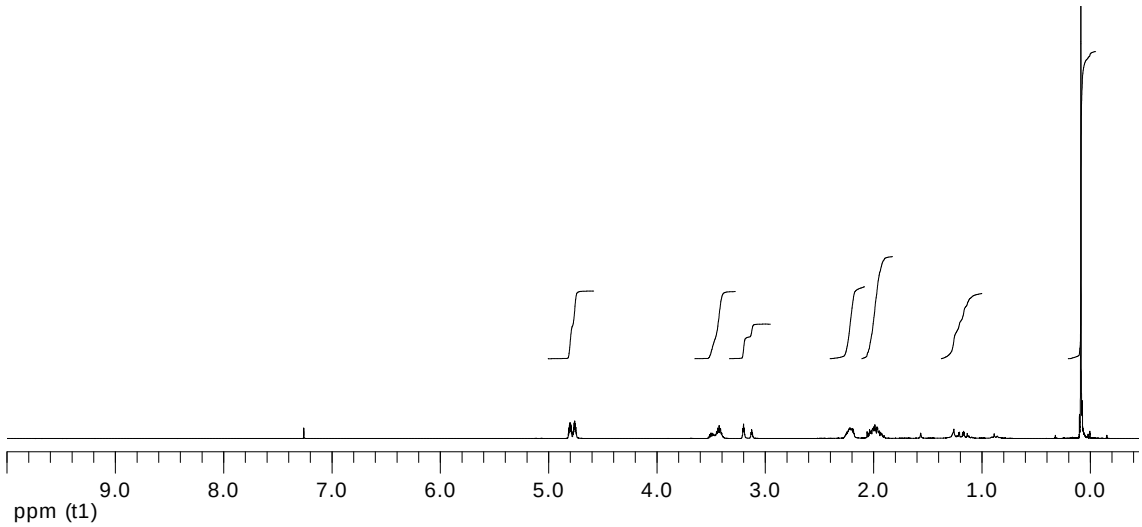


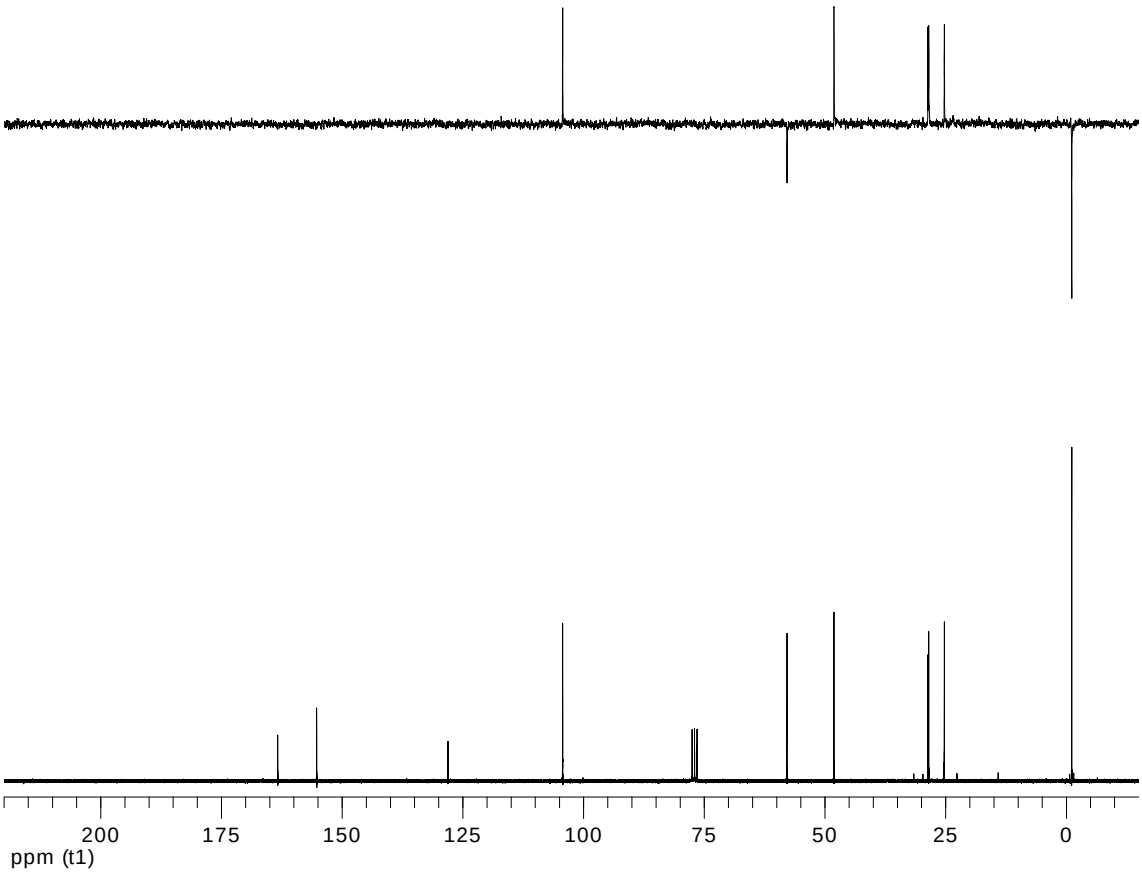
2a

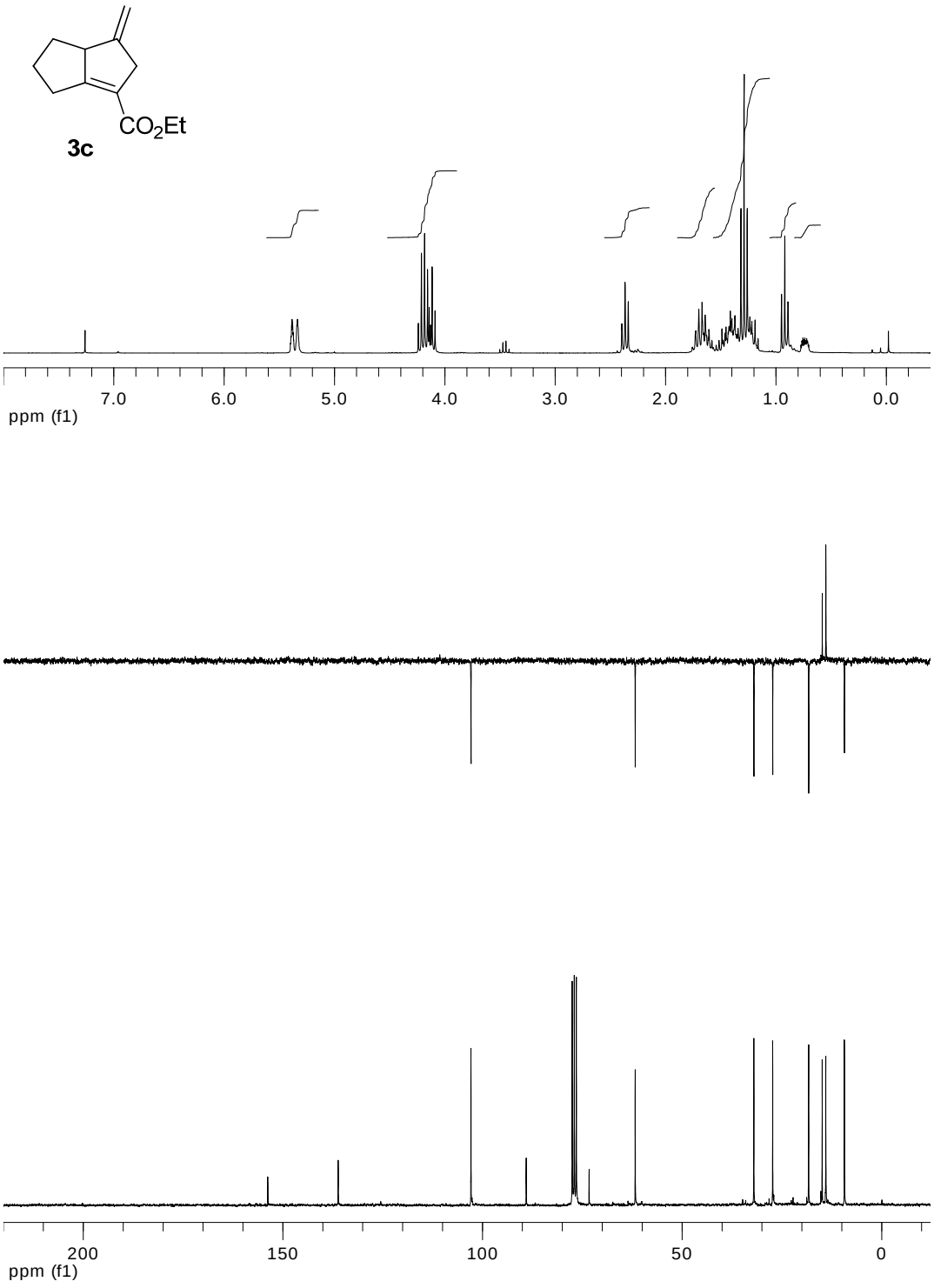




3a






CO2Et
3c
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)
200
150
100
50
0
ppm (f1)

3. Atomic Cartesian coordinates and computed energies (atomic units) for thestationary points calculated with basis set [B3LYP/6-31G(d) (C, H, O, P)LANL2DZ (Pd)

1*Z*

```
Zero-point correction=                           0.249108 (Hartree/Particle)
 Thermal correction to Energy=                    0.263817
 Thermal correction to Enthalpy=                  0.264761
 Thermal correction to Gibbs Free Energy=         0.204081
 Sum of electronic and zero-point Energies=           -578.919867
 Sum of electronic and thermal Energies=              -578.905159
 Sum of electronic and thermal Enthalpies=            -578.904215
 Sum of electronic and thermal Free Energies=         -578.964895
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.381307	-0.385820	-0.217933
2	6	0	5.338358	0.369937	0.605230
3	6	0	3.134244	-0.793591	-0.405262
4	6	0	5.780325	-0.381927	-0.664485
5	6	0	1.971778	-0.441246	0.485992
6	6	0	0.880525	0.361074	-0.248764
7	6	0	-0.332665	0.667865	0.654349
8	6	0	-1.344288	1.526905	-0.045695
9	6	0	-2.629926	1.257028	-0.330067
10	6	0	-3.349854	0.011010	0.015411
11	8	0	-2.913601	-0.969552	0.591453
12	8	0	-4.636142	0.091977	-0.414281
13	6	0	-5.445448	-1.058868	-0.141414
14	1	0	5.645887	-0.035042	1.568919
15	1	0	5.325543	1.459020	0.571838
16	1	0	2.911179	-1.420430	-1.270921
17	1	0	6.058283	0.211481	-1.535139
18	1	0	6.380099	-1.282967	-0.538977
19	1	0	2.332255	0.130805	1.350197
20	1	0	1.518923	-1.363011	0.882120
21	1	0	0.540259	-0.201003	-1.128697
22	1	0	1.314961	1.296754	-0.627114
23	1	0	-0.794109	-0.258427	1.000248
24	1	0	0.025268	1.215329	1.540585
25	1	0	-0.970318	2.496724	-0.380161
26	1	0	-3.228450	1.994311	-0.857030
27	1	0	-5.031398	-1.946909	-0.627528
28	1	0	-6.431807	-0.826606	-0.544867
29	1	0	-5.504775	-1.243633	0.934981

1*E*

```
Zero-point correction=                           0.248802 (Hartree/Particle)
 Thermal correction to Energy=                    0.263611
 Thermal correction to Enthalpy=                  0.264555
 Thermal correction to Gibbs Free Energy=         0.204267
 Sum of electronic and zero-point Energies=           -578.922906
 Sum of electronic and thermal Energies=              -578.908097
 Sum of electronic and thermal Enthalpies=            -578.907153
 Sum of electronic and thermal Free Energies=         -578.967440

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        4.630071    0.171764   -0.348367
    2          6             0        5.465979    0.498718    0.817382
    3          6             0        3.510925   -0.360929   -0.817372
    4          6             0        5.914373    0.830734   -0.618277
    5          6             0        2.421600   -0.958686    0.035013
    6          6             0        1.079317   -0.216532   -0.108870
    7          6             0       -0.049247   -0.863636    0.720649
    8          6             0       -1.338420   -0.105977    0.624136
    9          6             0       -2.491006   -0.589855    0.143146
   10          6             0       -3.702568    0.257449    0.082702
   11          8             0       -3.785062    1.417626    0.439259
   12          8             0       -4.747056   -0.436177   -0.435916
   13          6             0       -5.974279    0.297579   -0.539624
   14          1             0        5.985876   -0.303818    1.339757
   15          1             0        5.177494    1.327268    1.463550
   16          1             0        3.341369   -0.363235   -1.895898
   17          1             0        5.920484    1.878056   -0.918829
   18          1             0        6.730672    0.247777   -1.043730
   19          1             0        2.735473   -0.955632    1.086461
   20          1             0        2.271149   -2.012469   -0.247468
   21          1             0        0.780758   -0.192846   -1.165502
   22          1             0        1.209803    0.829444    0.198600
   23          1             0       -0.196178   -1.904019    0.403105
   24          1             0        0.267642   -0.895048    1.774662
   25          1             0       -1.331706    0.931015    0.961233
   26          1             0       -2.583882   -1.611464   -0.215638
   27          1             0       -6.308461    0.632888    0.446382
   28          1             0       -6.696131   -0.395841   -0.972983
   29          1             0       -5.847891    1.172558   -1.183549
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TS(1,2)*Z*

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Zero-point correction=                           0.300791 (Hartree/Particle)
 Thermal correction to Energy=                    0.324611
 Thermal correction to Enthalpy=                  0.325556
 Thermal correction to Gibbs Free Energy=         0.240037
 Sum of electronic and zero-point Energies=          -1391.920510
 Sum of electronic and thermal Energies=             -1391.896689
 Sum of electronic and thermal Enthalpies=           -1391.895745
 Sum of electronic and thermal Free Energies=        -1391.981264

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.654325   -1.117607   -0.404719
    2          6             0       -1.754389   -0.152253   -0.758146
```

3	6	0	-2.811008	-0.019176	0.355655
4	6	0	-3.974655	0.913069	-0.045321
5	6	0	-4.949250	1.099019	1.080062
6	6	0	-6.243366	0.741163	1.143168
7	6	0	0.629383	-0.795554	-0.280676
8	6	0	1.921390	-1.403342	0.027555
9	6	0	1.525088	0.354826	-0.396507
10	6	0	-7.010777	0.078541	0.065115
11	8	0	-6.611657	-0.267255	-1.032576
12	8	0	-8.293552	-0.114748	0.468719
13	6	0	-9.145813	-0.754616	-0.489458
14	1	0	-0.952097	-2.153340	-0.228321
15	1	0	-2.258988	-0.488253	-1.676855
16	1	0	-1.325407	0.833996	-0.978238
17	1	0	-2.327439	0.351854	1.269846
18	1	0	-3.215369	-1.010683	0.598971
19	1	0	-3.556523	1.898571	-0.303454
20	1	0	-4.482804	0.523015	-0.928511
21	1	0	-4.536471	1.573240	1.972674
22	1	0	-6.811690	0.940882	2.046838
23	1	0	2.104044	-1.692272	1.062514
24	1	0	2.346698	-2.074678	-0.717895
25	1	0	1.466810	1.114471	0.382538
26	1	0	1.718247	0.740346	-1.397458
27	1	0	-8.765947	-1.748775	-0.741839
28	1	0	-9.211584	-0.161209	-1.405875
29	1	0	-10.122869	-0.828503	-0.010361
30	46	0	3.817392	-0.010220	-0.004272
31	15	0	4.736583	2.159610	-0.250296
32	15	0	5.577246	-1.527376	0.459602
33	1	0	3.990413	3.335604	-0.562949
34	1	0	5.746219	2.416753	-1.218944
35	1	0	5.448226	2.769276	0.819988
36	1	0	5.415429	-2.930542	0.664457
37	1	0	6.415786	-1.352658	1.595484
38	1	0	6.655837	-1.678875	-0.455216

TS(1,2)*E*

Zero-point correction= 0.300330 (Hartree/Particle)
Thermal correction to Energy= 0.324315
Thermal correction to Enthalpy= 0.325259
Thermal correction to Gibbs Free Energy= 0.239280
Sum of electronic and zero-point Energies= -1391.923686
Sum of electronic and thermal Energies= -1391.899702
Sum of electronic and thermal Enthalpies= -1391.898758
Sum of electronic and thermal Free Energies= -1391.984737

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.245399	-2.098484	-0.377375
2	6	0	-1.403856	-1.656376	-1.231650
3	6	0	-2.685429	-1.402632	-0.414721
4	6	0	-3.883367	-1.000270	-1.299565
5	6	0	-5.142069	-0.807469	-0.510015
6	6	0	-5.844907	0.329981	-0.431190
7	6	0	0.892517	-1.426031	-0.236526
8	6	0	2.176260	-1.508638	0.455251

9	6	0	1.551901	-0.205434	-0.699605
10	6	0	-7.071900	0.407338	0.392102
11	8	0	-7.550540	-0.495041	1.052904
12	8	0	-7.619678	1.646707	0.320734
13	6	0	-8.817981	1.828038	1.086410
14	1	0	-0.370655	-3.034649	0.170642
15	1	0	-1.619899	-2.426622	-1.988775
16	1	0	-1.130871	-0.745994	-1.780789
17	1	0	-2.496983	-0.614989	0.325583
18	1	0	-2.941611	-2.306860	0.155067
19	1	0	-3.644033	-0.087346	-1.859941
20	1	0	-4.047755	-1.795157	-2.043828
21	1	0	-5.508169	-1.663043	0.058354
22	1	0	-5.549256	1.230142	-0.963480
23	1	0	2.175070	-1.337908	1.531627
24	1	0	2.879476	-2.266828	0.111832
25	1	0	1.176370	0.742005	-0.314108
26	1	0	1.883364	-0.178168	-1.737468
27	1	0	-8.627775	1.651880	2.148989
28	1	0	-9.598683	1.139447	0.750834
29	1	0	-9.121292	2.862154	0.918134
30	46	0	3.725929	0.226276	0.095069
31	15	0	4.245720	2.302393	-0.921755
32	15	0	5.583975	-0.466733	1.392395
33	1	0	3.374751	3.034468	-1.783592
34	1	0	5.373082	2.430966	-1.779660
35	1	0	4.578935	3.432911	-0.125395
36	1	0	5.641384	-1.665590	2.164584
37	1	0	6.090576	0.355013	2.437051
38	1	0	6.852926	-0.672881	0.783752

2Z

Zero-point correction= 0.303167 (Hartree/Particle)
Thermal correction to Energy= 0.326552
Thermal correction to Enthalpy= 0.327496
Thermal correction to Gibbs Free Energy= 0.244120
Sum of electronic and zero-point Energies= -1391.948632
Sum of electronic and thermal Energies= -1391.925247
Sum of electronic and thermal Enthalpies= -1391.924303
Sum of electronic and thermal Free Energies= -1392.007679

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-3.509612	-0.005942	0.039705
2	15	0	-4.361737	2.155909	-0.552762
3	6	0	-1.037448	-0.594638	0.687719
4	6	0	-1.702248	0.733729	0.865021
5	6	0	0.206578	-0.887596	0.272377
6	6	0	-2.212675	-1.512305	0.766700
7	6	0	1.325963	0.095876	0.056562
8	6	0	2.586723	-0.256172	0.869766
9	6	0	3.751939	0.724693	0.619289
10	6	0	4.940157	0.408499	1.477876
11	6	0	6.199705	0.113879	1.110697
12	15	0	-5.187106	-1.541846	-0.712297
13	6	0	6.706170	0.056619	-0.277460
14	8	0	6.093354	0.266582	-1.308849

15	8	0	8.024318	-0.280087	-0.270619
16	6	0	8.636678	-0.369109	-1.562391
17	1	0	-4.329846	3.157529	0.447331
18	1	0	-3.636409	2.880639	-1.529477
19	1	0	-5.654204	2.475646	-1.050819
20	1	0	-1.272519	1.589446	0.338813
21	1	0	-1.949761	0.983315	1.903183
22	1	0	0.442263	-1.933704	0.064606
23	1	0	-2.169869	-2.427576	0.169545
24	1	0	-2.567307	-1.710082	1.785046
25	1	0	0.997068	1.107997	0.326848
26	1	0	1.606011	0.138617	-1.008965
27	1	0	2.913415	-1.273740	0.615581
28	1	0	2.331234	-0.272198	1.938497
29	1	0	4.032328	0.727291	-0.435344
30	1	0	3.409096	1.740549	0.873860
31	1	0	4.739319	0.401239	2.551287
32	1	0	6.942119	-0.106862	1.872111
33	1	0	-4.817906	-2.435348	-1.746883
34	1	0	-5.610170	-2.529126	0.210028
35	1	0	-6.479963	-1.241198	-1.221306
36	1	0	8.145126	-1.132506	-2.172466
37	1	0	9.677064	-0.639574	-1.376831
38	1	0	8.577077	0.589238	-2.086357

2E

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Zero-point correction=                           0.302795 (Hartree/Particle)
 Thermal correction to Energy=                    0.326341
 Thermal correction to Enthalpy=                  0.327285
 Thermal correction to Gibbs Free Energy=         0.243483
 Sum of electronic and zero-point Energies=          -1391.952088
 Sum of electronic and thermal Energies=             -1391.928542
 Sum of electronic and thermal Enthalpies=           -1391.927598
 Sum of electronic and thermal Free Energies=        -1392.011400
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-3.660324	-0.039569	0.156022
2	15	0	-4.651463	2.123096	-0.150216
3	6	0	-1.102984	-0.583032	0.331246
4	6	0	-1.754968	0.710534	0.703224
5	6	0	0.052993	-0.814068	-0.314619
6	6	0	-2.224559	-1.541679	0.559965
7	6	0	1.093429	0.214422	-0.669538
8	6	0	2.476847	-0.110199	-0.072932
9	6	0	3.561174	0.908112	-0.484945
10	6	0	4.892998	0.613151	0.133586
11	6	0	6.014555	0.317090	-0.537313
12	15	0	-5.408720	-1.583815	-0.387159
13	6	0	7.273354	0.021881	0.179479
14	8	0	7.431559	0.019660	1.385941
15	8	0	8.271400	-0.257900	-0.698528
16	6	0	9.538181	-0.562083	-0.102298
17	1	0	-4.491130	3.058241	0.900609
18	1	0	-4.106442	2.935901	-1.173711
19	1	0	-6.013776	2.425239	-0.420955

20	1	0	-1.440702	1.610416	0.168918
21	1	0	-1.825795	0.888597	1.782282
22	1	0	0.271099	-1.839934	-0.619310
23	1	0	-2.265984	-2.421790	-0.087903
24	1	0	-2.391087	-1.804164	1.611160
25	1	0	0.778410	1.207142	-0.322333
26	1	0	1.200884	0.293108	-1.764616
27	1	0	2.788974	-1.114211	-0.390805
28	1	0	2.398110	-0.144843	1.021754
29	1	0	3.649933	0.935389	-1.578801
30	1	0	3.234928	1.910852	-0.167510
31	1	0	4.948274	0.622180	1.222620
32	1	0	6.044708	0.282199	-1.623097
33	1	0	-5.192764	-2.423325	-1.506716
34	1	0	-5.663351	-2.618825	0.544531
35	1	0	-6.770551	-1.292161	-0.671759
36	1	0	9.901403	0.284162	0.488079
37	1	0	10.214082	-0.766058	-0.933918
38	1	0	9.458636	-1.435988	0.550675

TS(2,3)*Z*

Zero-point correction= 0.302561 (Hartree/Particle)
Thermal correction to Energy= 0.325123
Thermal correction to Enthalpy= 0.326067
Thermal correction to Gibbs Free Energy= 0.245741
Sum of electronic and zero-point Energies= -1391.915816
Sum of electronic and thermal Energies= -1391.893254
Sum of electronic and thermal Enthalpies= -1391.892310
Sum of electronic and thermal Free Energies= -1391.972636

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.625758	-1.775287	0.329230
2	6	0	-1.974130	-1.727177	1.711835
3	6	0	-2.707101	-2.129900	-0.562537
4	6	0	-0.525693	-1.107918	-0.285912
5	46	0	-2.930892	-0.068811	-0.012286
6	15	0	-2.344724	1.967189	1.037106
7	6	0	0.647186	-0.602526	0.501638
8	6	0	1.669073	0.158523	-0.353545
9	6	0	2.892472	0.636255	0.455726
10	15	0	-4.828382	0.379280	-1.222901
11	6	0	3.836272	1.445774	-0.383765
12	6	0	5.136008	1.227208	-0.648115
13	6	0	5.948021	0.103597	-0.130970
14	8	0	5.597337	-0.792310	0.615595
15	8	0	7.214259	0.192283	-0.617991
16	6	0	8.105966	-0.844945	-0.191271
17	1	0	-1.254023	-1.401053	2.454232
18	1	0	-2.816065	-2.310558	2.066095
19	1	0	-3.531955	-2.727981	-0.181148
20	1	0	-2.502483	-2.239665	-1.625465
21	1	0	-0.383112	-1.272975	-1.350804
22	1	0	-2.947305	2.367601	2.255082
23	1	0	-2.465049	3.225109	0.390619
24	1	0	-1.001865	2.114648	1.460867
25	1	0	1.162100	-1.441756	1.008347

26	1	0	0.310853	0.049609	1.326362
27	1	0	1.173397	1.017164	-0.829409
28	1	0	2.013292	-0.489223	-1.171126
29	1	0	2.535730	1.276184	1.278984
30	1	0	3.412755	-0.212509	0.902397
31	1	0	-4.889255	0.053408	-2.602472
32	1	0	-5.299158	1.709675	-1.353152
33	1	0	-6.082450	-0.195673	-0.885222
34	1	0	3.391277	2.324245	-0.856044
35	1	0	5.674271	1.913619	-1.295206
36	1	0	7.739079	-1.825526	-0.507987
37	1	0	8.207913	-0.844167	0.897777
38	1	0	9.063009	-0.623294	-0.665353

TS(2,3)*E*

Zero-point correction= 0.302561 (Hartree/Particle)
Thermal correction to Energy= 0.325124
Thermal correction to Enthalpy= 0.326068
Thermal correction to Gibbs Free Energy= 0.246893
Sum of electronic and zero-point Energies= -1391.919285
Sum of electronic and thermal Energies= -1391.896723
Sum of electronic and thermal Enthalpies= -1391.895778
Sum of electronic and thermal Free Energies= -1391.974953

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.114991	1.877899	-0.223778
2	6	0	2.639277	2.171579	1.069599
3	6	0	3.108131	1.672839	-1.254991
4	6	0	0.825550	1.340395	-0.510721
5	46	0	2.974593	-0.116282	-0.081320
6	15	0	2.155107	-1.539201	1.622426
7	6	0	-0.301214	1.386484	0.477875
8	6	0	-1.548903	0.626958	0.007188
9	6	0	-2.727590	0.724662	0.997337
10	15	0	4.533563	-1.352112	-1.225778
11	6	0	-3.921858	-0.060958	0.548500
12	6	0	-5.129683	0.448712	0.272923
13	6	0	-6.235085	-0.421112	-0.184149
14	8	0	-6.181059	-1.625308	-0.350106
15	8	0	-7.358392	0.308125	-0.405801
16	6	0	-8.492716	-0.442210	-0.857508
17	1	0	1.982455	2.271417	1.926668
18	1	0	3.628086	2.606988	1.154081
19	1	0	4.085370	2.138434	-1.146570
20	1	0	2.781397	1.506038	-2.279277
21	1	0	0.570061	1.205783	-1.558582
22	1	0	2.855590	-1.693626	2.843874
23	1	0	1.908973	-2.921102	1.414045
24	1	0	0.898313	-1.220395	2.192199
25	1	0	-0.583175	2.435752	0.696095
26	1	0	0.022379	0.981297	1.451820
27	1	0	-1.289649	-0.428099	-0.156931
28	1	0	-1.869624	1.018442	-0.967603
29	1	0	-2.395651	0.341119	1.974932
30	1	0	-3.001806	1.776673	1.147564
31	1	0	4.434674	-1.487678	-2.634338
32	1	0	4.706549	-2.730009	-0.943995

33	1	0	5.912868	-1.014927	-1.208958
34	1	0	-3.790102	-1.135634	0.418085
35	1	0	-5.344503	1.509359	0.372209
36	1	0	-8.771419	-1.202468	-0.122209
37	1	0	-8.275073	-0.937270	-1.808322
38	1	0	-9.296831	0.284572	-0.980160

3*Z*

Zero-point correction= 0.303414 (Hartree/Particle)
Thermal correction to Energy= 0.326676
Thermal correction to Enthalpy= 0.327620
Thermal correction to Gibbs Free Energy= 0.245744
Sum of electronic and zero-point Energies= -1391.945081
Sum of electronic and thermal Energies= -1391.921819
Sum of electronic and thermal Enthalpies= -1391.920875
Sum of electronic and thermal Free Energies= -1392.002751

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.575021	2.059594	-0.215962
2	6	0	1.273157	3.100658	0.581763
3	6	0	2.894316	1.752022	-0.833585
4	6	0	0.842763	0.772603	-0.407579
5	46	0	2.715892	-0.254630	-0.161377
6	15	0	1.836293	-2.346689	0.598970
7	6	0	-0.363243	0.443741	0.456068
8	6	0	-1.640273	1.184351	0.002132
9	6	0	-2.849850	0.872667	0.910604
10	15	0	5.084200	-0.618809	-0.147484
11	6	0	-4.072463	1.628926	0.484164
12	6	0	-5.254760	1.152786	0.055720
13	6	0	-5.618856	-0.275141	-0.069545
14	8	0	-4.930423	-1.249547	0.177802
15	8	0	-6.895467	-0.383730	-0.524832
16	6	0	-7.372185	-1.724136	-0.691735
17	1	0	0.336699	3.162783	1.128680
18	1	0	1.984794	3.907255	0.740965
19	1	0	3.755965	2.318194	-0.470632
20	1	0	2.884899	1.676219	-1.926333
21	1	0	0.657736	0.564737	-1.469966
22	1	0	1.176632	-2.384010	1.851165
23	1	0	2.603916	-3.525808	0.787282
24	1	0	0.798290	-2.951686	-0.149542
25	1	0	-0.148236	0.699224	1.502795
26	1	0	-0.581083	-0.633639	0.429937
27	1	0	-1.880044	0.888802	-1.027952
28	1	0	-1.453960	2.264897	-0.020374
29	1	0	-3.051024	-0.199839	0.922597
30	1	0	-2.598202	1.179614	1.937986
31	1	0	5.775075	-0.319417	-1.346220
32	1	0	5.791108	-1.818221	0.143630
33	1	0	5.850309	0.221517	0.695944
34	1	0	-3.971343	2.715759	0.508256
35	1	0	-6.039547	1.846317	-0.231718
36	1	0	-7.352476	-2.263498	0.259688

37	1	0	-6.756701	-2.266990	-1.414959
38	1	0	-8.395864	-1.628957	-1.056228

3*E*

Zero-point correction= 0.303120 (Hartree/Particle)
Thermal correction to Energy= 0.326495
Thermal correction to Enthalpy= 0.327439
Thermal correction to Gibbs Free Energy= 0.245827
Sum of electronic and zero-point Energies= -1391.947762
Sum of electronic and thermal Energies= -1391.924387
Sum of electronic and thermal Enthalpies= -1391.923443
Sum of electronic and thermal Free Energies= -1392.005055

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.374442	1.905215	0.007866
2	6	0	0.877522	2.765941	0.914813
3	6	0	2.713673	1.955212	-0.640741
4	6	0	0.928477	0.518850	-0.323502
5	46	0	2.984253	-0.103717	-0.201574
6	15	0	2.599080	-2.407924	0.313378
7	6	0	-0.157637	-0.148210	0.504000
8	6	0	-1.573839	0.346325	0.136035
9	6	0	-2.668473	-0.286024	1.021945
10	15	0	5.375276	0.056488	-0.230989
11	6	0	-4.041638	0.203378	0.677285
12	6	0	-5.053878	-0.561231	0.246094
13	6	0	-6.368822	0.031312	-0.080490
14	8	0	-6.668496	1.207382	0.002946
15	8	0	-7.235530	-0.926522	-0.499835
16	6	0	-8.544205	-0.453967	-0.842967
17	1	0	-0.038127	2.569266	1.465095
18	1	0	1.404156	3.685154	1.159548
19	1	0	3.445107	2.647137	-0.215475
20	1	0	2.694439	2.001213	-1.734962
21	1	0	0.761342	0.392208	-1.401540
22	1	0	2.033349	-2.734215	1.569939
23	1	0	3.601413	-3.412996	0.325749
24	1	0	1.667504	-3.126684	-0.474186
25	1	0	0.026349	0.038346	1.570983
26	1	0	-0.140630	-1.239350	0.364704
27	1	0	-1.779063	0.106390	-0.915760
28	1	0	-1.618176	1.438468	0.217782
29	1	0	-2.626978	-1.380598	0.943855
30	1	0	-2.453384	-0.033755	2.071906
31	1	0	5.954540	0.643910	-1.381146
32	1	0	6.330981	-0.987224	-0.090317
33	1	0	5.961043	0.933232	0.713553
34	1	0	-4.225331	1.274098	0.770646
35	1	0	-4.952696	-1.636211	0.122159
36	1	0	-8.490719	0.278864	-1.653162
37	1	0	-9.025497	0.013455	0.020967
38	1	0	-9.102109	-1.335886	-1.160670

2*Z´*

Zero-point correction= 0.276013 (Hartree/Particle)
Thermal correction to Energy= 0.295254
Thermal correction to Enthalpy= 0.296199
Thermal correction to Gibbs Free Energy= 0.225504
Sum of electronic and zero-point Energies= -1048.813444
Sum of electronic and thermal Energies= -1048.794203
Sum of electronic and thermal Enthalpies= -1048.793258
Sum of electronic and thermal Free Energies= -1048.863953

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.225884	-0.480313	-0.305948
2	6	0	-0.914685	-1.824235	-0.715914
3	6	0	-0.441798	-0.700694	-1.572744
4	6	0	-2.128642	-2.035951	-0.168587
5	6	0	0.392053	-2.395759	-0.298621
6	6	0	-3.394447	-1.310000	-0.541998
7	6	0	-3.987378	-0.381567	0.543366
8	6	0	-3.195128	0.917973	0.802014
9	6	0	-1.914013	0.725473	1.556370
10	6	0	-0.698449	1.259505	1.319467
11	15	0	3.137157	-0.736742	1.135736
12	6	0	-0.363526	2.130498	0.180306
13	8	0	-1.111805	2.800241	-0.501099
14	8	0	1.002315	2.111940	-0.056936
15	6	0	1.438638	2.957767	-1.136478
16	1	0	-1.060593	0.195778	-1.639069
17	1	0	-0.035802	-1.001330	-2.544396
18	1	0	-2.222853	-2.813371	0.592318
19	1	0	0.464347	-2.861987	0.687363
20	1	0	0.928535	-2.955364	-1.070521
21	1	0	-4.170418	-2.052060	-0.787561
22	1	0	-3.235196	-0.724691	-1.457106
23	1	0	-4.093584	-0.939891	1.485371
24	1	0	-5.004430	-0.096501	0.241011
25	1	0	-3.017561	1.460860	-0.129622
26	1	0	-3.829833	1.574696	1.420047
27	1	0	-1.990073	0.074428	2.428419
28	1	0	0.130807	1.009276	1.973510
29	1	0	3.056057	-0.540708	2.539285
30	1	0	3.739888	-2.016079	1.195770
31	1	0	4.340425	-0.005553	0.954826
32	1	0	1.131957	3.990865	-0.955826
33	1	0	1.014585	2.616424	-2.084145
34	1	0	2.525896	2.875224	-1.150885

$2Z_t'$

Zero-point correction= 0.275663 (Hartree/Particle)
Thermal correction to Energy= 0.295207
Thermal correction to Enthalpy= 0.296151
Thermal correction to Gibbs Free Energy= 0.224940
Sum of electronic and zero-point Energies= -1048.812009
Sum of electronic and thermal Energies= -1048.792465
Sum of electronic and thermal Enthalpies= -1048.791521
Sum of electronic and thermal Free Energies= -1048.862732

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	46	0	-1.574488	-1.112738	-0.275559
2	15	0	-2.948888	0.343507	1.083633
3	6	0	0.869571	-2.125632	-0.214368
4	6	0	0.033994	-1.670122	0.930927
5	6	0	2.197665	-2.062510	-0.388266
6	6	0	-0.217304	-2.380432	-1.213687
7	6	0	3.199413	-1.606541	0.640340
8	6	0	4.078433	-0.423868	0.177204
9	6	0	3.296930	0.849683	-0.192216
10	6	0	2.567092	1.458923	0.972009
11	6	0	1.408037	2.141959	0.968764
12	6	0	0.614724	2.449004	-0.239193
13	8	0	0.929616	2.257564	-1.398475
14	8	0	-0.570034	3.030844	0.108199
15	6	0	-1.385205	3.440466	-0.998186
16	1	0	-4.080827	-0.172433	1.765075
17	1	0	-2.330690	0.925294	2.214473
18	1	0	-3.579316	1.527337	0.621735
19	1	0	0.358914	-0.798592	1.501855
20	1	0	-0.386686	-2.462188	1.558312
21	1	0	2.599794	-2.345687	-1.363294
22	1	0	-0.024302	-2.042708	-2.237216
23	1	0	-0.654873	-3.384745	-1.177505
24	1	0	3.873494	-2.438647	0.897724
25	1	0	2.681963	-1.338893	1.570710
26	1	0	4.660737	-0.733282	-0.700981
27	1	0	4.810478	-0.192760	0.965116
28	1	0	4.008977	1.599734	-0.572374
29	1	0	2.599789	0.657277	-1.010149
30	1	0	3.050755	1.335343	1.943549
31	1	0	1.000716	2.522266	1.901205
32	1	0	-0.841588	4.139870	-1.639371
33	1	0	-2.257160	3.926363	-0.557509
34	1	0	-1.687175	2.576952	-1.597890

2E´

Zero-point correction= 0.275673 (Hartree/Particle)
Thermal correction to Energy= 0.295087
Thermal correction to Enthalpy= 0.296031
Thermal correction to Gibbs Free Energy= 0.224819
Sum of electronic and zero-point Energies= -1048.815171
Sum of electronic and thermal Energies= -1048.795757
Sum of electronic and thermal Enthalpies= -1048.794813
Sum of electronic and thermal Free Energies= -1048.866024

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.290039	-0.522974	-0.386060
2	15	0	-2.776512	-1.241466	1.370409
3	6	0	0.928981	-1.266870	-1.410259
4	6	0	-0.046092	-2.164143	-0.735363
5	6	0	2.248483	-1.080155	-1.195718
6	6	0	-0.004532	-0.297638	-2.039737
7	6	0	3.127025	-1.810615	-0.218305
8	6	0	3.837587	-0.857153	0.768283

9	6	0	2.901571	-0.048861	1.694959
10	6	0	2.043795	0.972119	1.003056
11	6	0	0.727530	1.143886	1.226411
12	6	0	-0.129160	2.089231	0.494767
13	8	0	-1.351798	1.973905	0.389972
14	8	0	0.541722	3.108257	-0.076295
15	6	0	-0.244088	4.001189	-0.882068
16	1	0	-2.909153	-2.622510	1.655620
17	1	0	-2.666324	-0.815406	2.720274
18	1	0	-4.162919	-0.973107	1.241901
19	1	0	0.240407	-2.649967	0.200332
20	1	0	-0.592358	-2.837572	-1.401674
21	1	0	2.725074	-0.257623	-1.733120
22	1	0	0.359323	0.723449	-2.185576
23	1	0	-0.581208	-0.668619	-2.893349
24	1	0	3.912701	-2.379668	-0.741618
25	1	0	2.544494	-2.550354	0.346999
26	1	0	4.461805	-0.153727	0.197979
27	1	0	4.527833	-1.433825	1.399155
28	1	0	2.269737	-0.730323	2.279777
29	1	0	3.537847	0.483456	2.420638
30	1	0	2.543936	1.628473	0.293109
31	1	0	0.188309	0.489581	1.904722
32	1	0	-1.017033	4.483611	-0.278534
33	1	0	-0.719032	3.459326	-1.704302
34	1	0	0.460069	4.740359	-1.265302

$2E_t'$

Zero-point correction= 0.276058 (Hartree/Particle)
Thermal correction to Energy= 0.295381
Thermal correction to Enthalpy= 0.296325
Thermal correction to Gibbs Free Energy= 0.226082
Sum of electronic and zero-point Energies= -1048.814730
Sum of electronic and thermal Energies= -1048.795407
Sum of electronic and thermal Enthalpies= -1048.794463
Sum of electronic and thermal Free Energies= -1048.864706

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.213604	-1.383654	-0.328179
2	15	0	-0.898684	-2.497398	1.691452
3	6	0	1.951075	-0.475800	-1.244515
4	6	0	1.869236	-1.640640	-0.323268
5	6	0	2.583543	0.710817	-1.116640
6	6	0	0.747822	-0.722528	-2.082064
7	6	0	3.446427	1.188287	0.020237
8	6	0	2.901734	2.487120	0.661509
9	6	0	1.632479	2.352241	1.546137
10	6	0	0.440390	1.709409	0.899365
11	6	0	-0.721207	2.319244	0.606937
12	6	0	-1.867262	1.605462	0.012595
13	8	0	-1.959761	0.414631	-0.276840
14	8	0	-2.896712	2.456260	-0.191764
15	6	0	-4.076732	1.889445	-0.778484
16	1	0	-1.613355	-3.716016	1.570679
17	1	0	0.101035	-2.993220	2.564201
18	1	0	-1.724036	-1.941917	2.706584

19	1	0	2.278441	-1.553474	0.686204
20	1	0	2.096616	-2.606144	-0.781365
21	1	0	2.350163	1.470725	-1.865610
22	1	0	0.253500	0.146877	-2.522419
23	1	0	0.794328	-1.581909	-2.757714
24	1	0	4.466981	1.411441	-0.331148
25	1	0	3.557485	0.410326	0.788287
26	1	0	2.693850	3.210679	-0.138423
27	1	0	3.680628	2.938079	1.291804
28	1	0	1.898677	1.748331	2.427520
29	1	0	1.361532	3.349455	1.916535
30	1	0	0.516927	0.646814	0.677884
31	1	0	-0.877485	3.377797	0.798035
32	1	0	-3.850997	1.456366	-1.756725
33	1	0	-4.778219	2.718265	-0.878872
34	1	0	-4.493280	1.111115	-0.133033

TS(2,3)*Z´*

Zero-point correction= 0.276104 (Hartree/Particle)
Thermal correction to Energy= 0.294360
Thermal correction to Enthalpy= 0.295304
Thermal correction to Gibbs Free Energy= 0.229258
Sum of electronic and zero-point Energies= -1048.786959
Sum of electronic and thermal Energies= -1048.768703
Sum of electronic and thermal Enthalpies= -1048.767759
Sum of electronic and thermal Free Energies= -1048.833804

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.530199	1.050698	1.367768
2	6	0	2.419972	-0.090113	1.425518
3	6	0	0.301034	0.800959	2.063770
4	6	0	1.742850	1.958288	0.297447
5	46	0	0.820844	-0.506540	0.053935
6	6	0	0.850917	3.112551	-0.039079
7	15	0	1.678076	-2.481805	-0.776906
8	6	0	-1.213652	-0.527316	-1.049321
9	6	0	-0.481718	0.441488	-1.733496
10	6	0	-0.702457	1.937548	-1.787669
11	6	0	-0.589443	2.810162	-0.522173
12	6	0	-2.370048	-0.267988	-0.162576
13	8	0	-2.879339	0.810254	0.090064
14	8	0	-2.873768	-1.441472	0.303827
15	6	0	-4.011693	-1.314903	1.163514
16	1	0	3.381139	-0.046000	0.916989
17	1	0	2.379733	-0.742931	2.293901
18	1	0	0.326059	0.152018	2.932811
19	1	0	-0.540524	1.478174	1.990656
20	1	0	2.722725	1.925226	-0.169950
21	1	0	1.348265	3.725773	-0.801897
22	1	0	0.734542	3.763030	0.847133
23	1	0	1.706438	-3.658951	0.014154
24	1	0	1.091439	-3.078665	-1.922950
25	1	0	3.024256	-2.569422	-1.217955
26	1	0	-1.164935	-1.552607	-1.402211
27	1	0	0.132097	0.055095	-2.544029
28	1	0	-0.033962	2.343271	-2.557160

29	1	0	-1.730138	2.071188	-2.157847
30	1	0	-1.066132	3.774030	-0.749413
31	1	0	-1.188227	2.359896	0.268103
32	1	0	-4.832312	-0.804325	0.651305
33	1	0	-3.752958	-0.750513	2.064316
34	1	0	-4.298384	-2.334884	1.423287

TS(2,3)Z_t'

Zero-point correction= 0.275881 (Hartree/Particle)
Thermal correction to Energy= 0.294178
Thermal correction to Enthalpy= 0.295122
Thermal correction to Gibbs Free Energy= 0.229174
Sum of electronic and zero-point Energies= -1048.784296
Sum of electronic and thermal Energies= -1048.765999
Sum of electronic and thermal Enthalpies= -1048.765055
Sum of electronic and thermal Free Energies= -1048.831003

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.580132	-0.761391	0.192502
2	6	0	2.074273	-1.976922	-0.410901
3	6	0	2.485180	-0.773512	1.622254
4	6	0	2.663054	0.361144	-0.681123
5	46	0	0.404218	-0.772158	0.139650
6	6	0	2.935185	1.766339	-0.244132
7	15	0	-1.223432	-2.083341	-0.827960
8	6	0	-1.057786	0.888237	1.008840
9	6	0	0.115066	1.546624	0.693502
10	6	0	0.393965	2.418719	-0.503620
11	6	0	1.877390	2.817841	-0.688406
12	6	0	-2.297156	0.981077	0.203461
13	8	0	-2.438224	1.546920	-0.864590
14	8	0	-3.319634	0.343862	0.836618
15	6	0	-4.593502	0.431322	0.183327
16	1	0	2.124500	-2.099232	-1.491276
17	1	0	2.096994	-2.899425	0.164552
18	1	0	2.545490	-1.726007	2.136240
19	1	0	2.734775	0.105179	2.207978
20	1	0	2.653287	0.155215	-1.748768
21	1	0	3.907247	2.121096	-0.627461
22	1	0	3.029506	1.798111	0.847762
23	1	0	-1.940873	-3.053237	-0.082384
24	1	0	-2.347297	-1.485414	-1.449424
25	1	0	-0.863312	-2.937657	-1.898235
26	1	0	-1.180340	0.477059	2.005601
27	1	0	0.849099	1.573243	1.495723
28	1	0	-0.003071	1.935670	-1.397553
29	1	0	-0.202015	3.339039	-0.394609
30	1	0	2.025077	3.051752	-1.750174
31	1	0	2.083050	3.750510	-0.145560
32	1	0	-4.558141	-0.033767	-0.806158
33	1	0	-4.897150	1.475560	0.068585
34	1	0	-5.291339	-0.101420	0.830234

TS(2,3)*E*´

Zero-point correction= 0.276760 (Hartree/Particle)
Thermal correction to Energy= 0.294642
Thermal correction to Enthalpy= 0.295586
Thermal correction to Gibbs Free Energy= 0.231389
Sum of electronic and zero-point Energies= -1048.794797
Sum of electronic and thermal Energies= -1048.776915
Sum of electronic and thermal Enthalpies= -1048.775971
Sum of electronic and thermal Free Energies= -1048.840168

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.285656	-0.737070	0.967707
2	6	0	1.803074	-2.074030	0.683151
3	6	0	1.671498	-0.151736	2.114448
4	6	0	2.847082	-0.044111	-0.138768
5	46	0	0.334252	-0.657270	0.040330
6	6	0	3.213841	1.408497	-0.137321
7	15	0	-1.103068	-2.150767	-1.008383
8	6	0	-0.897623	1.294786	0.008630
9	6	0	-0.121692	1.315843	-1.144850
10	6	0	1.065825	2.224498	-1.367485
11	6	0	2.055104	2.444532	-0.209258
12	6	0	-2.312951	0.871909	-0.029128
13	8	0	-2.879643	0.304886	-0.952848
14	8	0	-2.951252	1.229295	1.110922
15	6	0	-4.337773	0.873394	1.179129
16	1	0	2.220982	-2.624129	-0.157537
17	1	0	1.437007	-2.686249	1.503950
18	1	0	1.340121	-0.795554	2.921155
19	1	0	1.812444	0.896851	2.352196
20	1	0	3.212414	-0.656837	-0.957121
21	1	0	3.880051	1.601016	-0.988071
22	1	0	3.794276	1.653924	0.768834
23	1	0	-2.401067	-2.414050	-0.514373
24	1	0	-1.466702	-1.961599	-2.361948
25	1	0	-0.673986	-3.495800	-1.123433
26	1	0	-0.601194	1.846104	0.893574
27	1	0	-0.587411	0.925922	-2.047130
28	1	0	1.610137	1.890330	-2.258594
29	1	0	0.634315	3.205426	-1.630749
30	1	0	2.508917	3.438117	-0.320871
31	1	0	1.512697	2.470112	0.742354
32	1	0	-4.461622	-0.211901	1.121392
33	1	0	-4.897975	1.336579	0.362087
34	1	0	-4.688054	1.245128	2.142752

TS(2,3)E_t´

Zero-point correction= 0.275561 (Hartree/Particle)
Thermal correction to Energy= 0.294037
Thermal correction to Enthalpy= 0.294982
Thermal correction to Gibbs Free Energy= 0.228322
Sum of electronic and zero-point Energies= -1048.786172
Sum of electronic and thermal Energies= -1048.767695
Sum of electronic and thermal Enthalpies= -1048.766751
Sum of electronic and thermal Free Energies= -1048.833411

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.032183	0.861948	1.147825
2	6	0	-1.548444	2.171596	0.770188
3	6	0	-1.294133	0.300718	2.238244
4	6	0	-2.789193	0.179844	0.149747
5	46	0	-0.207796	0.695756	-0.012330
6	6	0	-3.176699	-1.262599	0.232908
7	15	0	1.158046	2.157288	-1.158989
8	6	0	1.002711	-1.168145	-0.713959
9	6	0	-0.247978	-1.672191	-0.433643
10	6	0	-1.295765	-1.974093	-1.475141
11	6	0	-2.749665	-2.145253	-0.972183
12	6	0	2.116410	-1.291296	0.264118
13	8	0	2.076072	-1.862138	1.334372
14	8	0	3.241537	-0.700071	-0.223675
15	6	0	4.382887	-0.765556	0.642913
16	1	0	-2.037315	2.712081	-0.038198
17	1	0	-1.062227	2.790614	1.520355
18	1	0	-0.833509	0.969500	2.955766
19	1	0	-1.438536	-0.725693	2.555647
20	1	0	-3.238439	0.788525	-0.631226
21	1	0	-4.270271	-1.378009	0.328465
22	1	0	-2.758406	-1.697880	1.147699
23	1	0	2.254788	2.775057	-0.505868
24	1	0	1.874580	1.739334	-2.307831
25	1	0	0.617072	3.345138	-1.712090
26	1	0	1.285115	-0.918853	-1.733175
27	1	0	-0.385339	-2.075625	0.567845
28	1	0	-1.243494	-1.209764	-2.256739
29	1	0	-1.005217	-2.921833	-1.958655
30	1	0	-3.414838	-1.948550	-1.822688
31	1	0	-2.920043	-3.194729	-0.696173
32	1	0	4.631146	-1.804147	0.877306
33	1	0	4.187164	-0.230029	1.576503
34	1	0	5.197157	-0.291372	0.093381

3Z´

Zero-point correction= 0.276870 (Hartree/Particle)
Thermal correction to Energy= 0.295635
Thermal correction to Enthalpy= 0.296579
Thermal correction to Gibbs Free Energy= 0.229487
Sum of electronic and zero-point Energies= -1048.824549
Sum of electronic and thermal Energies= -1048.805784
Sum of electronic and thermal Enthalpies= -1048.804840
Sum of electronic and thermal Free Energies= -1048.871932

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.418176	-0.511695	-0.144972
2	15	0	-1.091498	-2.365313	0.128925
3	6	0	3.051305	-0.733262	0.117463
4	6	0	2.003342	-1.506930	0.828719
5	6	0	2.313770	0.517822	-0.250758

6	6	0	4.242555	-1.144426	-0.335438
7	6	0	-0.249020	1.612088	-0.942306
8	6	0	-1.361375	0.798135	-1.037700
9	6	0	2.392398	1.697454	0.710751
10	6	0	-2.473609	0.778996	-0.061572
11	8	0	-2.562273	1.407838	0.975956
12	8	0	-3.460362	-0.060494	-0.492909
13	6	0	-4.626359	-0.106976	0.342136
14	6	0	1.569748	2.912945	0.261970
15	6	0	0.064319	2.635146	0.120698
16	1	0	-2.164300	-2.359277	1.054356
17	1	0	-1.818675	-2.886720	-0.968566
18	1	0	-0.511380	-3.584572	0.550388
19	1	0	1.839924	-1.213560	1.872047
20	1	0	2.022060	-2.593690	0.713056
21	1	0	2.500606	0.828196	-1.285478
22	1	0	4.861055	-0.508391	-0.965333
23	1	0	4.623521	-2.139207	-0.113519
24	1	0	0.344908	1.696430	-1.850788
25	1	0	-1.565677	0.294370	-1.977652
26	1	0	3.448305	2.005579	0.797092
27	1	0	2.085706	1.390803	1.720228
28	1	0	-5.073996	0.886435	0.433000
29	1	0	-4.375327	-0.470917	1.342576
30	1	0	-5.314750	-0.792556	-0.153473
31	1	0	1.708704	3.734865	0.975363
32	1	0	1.961592	3.272508	-0.701793
33	1	0	-0.439986	3.570888	-0.170281
34	1	0	-0.377276	2.341789	1.075454

$3Z_t'$

Zero-point correction= 0.276785 (Hartree/Particle)
Thermal correction to Energy= 0.295739
Thermal correction to Enthalpy= 0.296684
Thermal correction to Gibbs Free Energy= 0.228770
Sum of electronic and zero-point Energies= -1048.822027
Sum of electronic and thermal Energies= -1048.803073
Sum of electronic and thermal Enthalpies= -1048.802129
Sum of electronic and thermal Free Energies= -1048.870043

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.924446	-0.792395	-0.453947
2	6	0	1.877601	-1.801641	-0.762447
3	6	0	4.133875	-0.989528	0.096035
4	6	0	2.152981	0.473726	-0.582705
5	46	0	0.364774	-0.576971	0.053268
6	6	0	2.627307	1.704883	0.159579
7	15	0	-1.151682	-2.434549	0.303694
8	6	0	-1.326972	0.827509	0.993949
9	6	0	-0.167321	1.571024	0.971885
10	6	0	0.217861	2.650911	-0.006110
11	6	0	1.733591	2.948770	-0.010874
12	6	0	-2.409272	0.925170	-0.012544
13	8	0	-2.438569	1.636060	-0.998295
14	8	0	-3.431607	0.084899	0.317883
15	6	0	-4.557339	0.118136	-0.572096

16	1	0	1.615169	-1.886114	-1.822845
17	1	0	1.969863	-2.779097	-0.282570
18	1	0	4.523161	-1.992383	0.253816
19	1	0	4.758421	-0.163600	0.424275
20	1	0	1.867675	0.680863	-1.622919
21	1	0	3.642848	1.962403	-0.183776
22	1	0	2.739727	1.456327	1.223484
23	1	0	-1.988621	-2.648841	1.427686
24	1	0	-2.140497	-2.657449	-0.684789
25	1	0	-0.577678	-3.726875	0.267209
26	1	0	-1.579208	0.271163	1.890970
27	1	0	0.433340	1.523234	1.879757
28	1	0	-0.142593	2.391660	-1.002316
29	1	0	-0.327784	3.566303	0.270568
30	1	0	1.972981	3.452439	-0.955676
31	1	0	1.975322	3.666198	0.784376
32	1	0	-4.265272	-0.195703	-1.578309
33	1	0	-4.975094	1.126989	-0.625675
34	1	0	-5.285299	-0.575695	-0.150071

3*E´*

Zero-point correction= 0.276791 (Hartree/Particle)
Thermal correction to Energy= 0.295681
Thermal correction to Enthalpy= 0.296625
Thermal correction to Gibbs Free Energy= 0.228950
Sum of electronic and zero-point Energies= -1048.827922
Sum of electronic and thermal Energies= -1048.809033
Sum of electronic and thermal Enthalpies= -1048.808088
Sum of electronic and thermal Free Energies= -1048.875764

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.310334	-0.491480	-0.238955
2	15	0	1.066049	-2.303840	-1.038931
3	6	0	-2.609215	-0.809201	1.039344
4	6	0	-2.000054	-1.722642	0.038877
5	6	0	-1.982674	0.504387	0.681084
6	6	0	-3.299985	-1.110478	2.146426
7	6	0	0.388230	1.770278	-0.361729
8	6	0	1.439573	0.994667	-0.796903
9	6	0	-2.724636	1.395404	-0.308466
10	6	0	2.592699	0.593231	0.041138
11	8	0	3.519798	-0.087294	-0.365989
12	8	0	2.520072	1.057874	1.310102
13	6	0	3.597735	0.665079	2.172213
14	6	0	-1.975762	2.691153	-0.649419
15	6	0	-0.582656	2.482379	-1.268715
16	1	0	1.898769	-2.236227	-2.181913
17	1	0	2.023922	-2.857157	-0.158161
18	1	0	0.402143	-3.509620	-1.366496
19	1	0	-2.464200	-1.698155	-0.953816
20	1	0	-1.795604	-2.747460	0.360328
21	1	0	-1.646133	1.068665	1.558621
22	1	0	-3.571931	-0.346288	2.871659
23	1	0	-3.588603	-2.134040	2.376505
24	1	0	0.402566	2.093341	0.675972
25	1	0	1.583800	0.797518	-1.855576

26	1	0	-3.700875	1.668371	0.127211
27	1	0	-2.953017	0.840848	-1.229217
28	1	0	4.554770	1.016424	1.777483
29	1	0	3.633274	-0.423240	2.273346
30	1	0	3.385045	1.130270	3.135160
31	1	0	-2.578506	3.297051	-1.337667
32	1	0	-1.863403	3.288531	0.267637
33	1	0	-0.156257	3.473310	-1.493816
34	1	0	-0.659618	1.953372	-2.227364

$3E_t'$

Zero-point correction= 0.276840 (Hartree/Particle)
Thermal correction to Energy= 0.295718
Thermal correction to Enthalpy= 0.296662
Thermal correction to Gibbs Free Energy= 0.229365
Sum of electronic and zero-point Energies= -1048.823276
Sum of electronic and thermal Energies= -1048.804398
Sum of electronic and thermal Enthalpies= -1048.803453
Sum of electronic and thermal Free Energies= -1048.870751

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.745872	-1.140045	0.501520
2	6	0	1.742262	-2.073123	-0.073091
3	6	0	3.535506	-1.319362	1.572795
4	6	0	2.388105	0.124507	-0.194877
5	46	0	0.318805	-0.525383	-0.272206
6	6	0	2.761803	1.452125	0.425113
7	15	0	-1.461178	-2.119369	-0.580064
8	6	0	-1.257718	1.243431	-0.502731
9	6	0	-0.087124	1.827318	-0.080783
10	6	0	0.880309	2.561784	-0.970753
11	6	0	2.306114	2.679879	-0.383968
12	6	0	-2.340260	0.971623	0.474041
13	8	0	-2.286484	1.145744	1.675280
14	8	0	-3.455415	0.507380	-0.157297
15	6	0	-4.588288	0.284012	0.696395
16	1	0	1.943588	-2.396294	-1.100481
17	1	0	1.408434	-2.900400	0.558627
18	1	0	3.598158	-2.283983	2.070274
19	1	0	4.117052	-0.507981	2.001160
20	1	0	2.614700	0.076982	-1.268984
21	1	0	3.857484	1.502971	0.537403
22	1	0	2.363343	1.497689	1.447182
23	1	0	-2.453788	-2.359529	0.401972
24	1	0	-2.332616	-2.062240	-1.694669
25	1	0	-1.053817	-3.463902	-0.741805
26	1	0	-1.524042	1.199715	-1.555444
27	1	0	0.006538	1.987651	0.992641
28	1	0	0.900015	2.086753	-1.957763
29	1	0	0.483873	3.576493	-1.131049
30	1	0	3.001048	2.859117	-1.213901
31	1	0	2.364945	3.567637	0.258537
32	1	0	-4.882583	1.212231	1.193507
33	1	0	-4.358846	-0.465069	1.459372
34	1	0	-5.385143	-0.067571	0.040023

TS(3,4)Z´

Zero-point correction= 0.277634 (Hartree/Particle)
Thermal correction to Energy= 0.295400
Thermal correction to Enthalpy= 0.296345
Thermal correction to Gibbs Free Energy= 0.230519
Sum of electronic and zero-point Energies= -1048.789370
Sum of electronic and thermal Energies= -1048.771604
Sum of electronic and thermal Enthalpies= -1048.770660
Sum of electronic and thermal Free Energies= -1048.836485

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.235097	-0.807363	0.008413
2	15	0	1.212184	-2.370669	-0.687491
3	6	0	-2.543891	-0.698316	0.397436
4	6	0	-2.081863	-1.539772	-0.722389
5	6	0	-2.137289	0.774948	0.354526
6	6	0	-3.113481	-1.205444	1.523068
7	6	0	-0.397391	1.577815	0.731453
8	6	0	0.841906	0.775355	0.973794
9	6	0	-2.529420	1.582187	-0.879614
10	6	0	2.083952	0.974712	0.222292
11	8	0	2.238400	1.453042	-0.894419
12	8	0	3.153893	0.492153	0.938818
13	6	0	4.424438	0.640204	0.300181
14	6	0	-1.860251	2.952661	-0.740070
15	6	0	-0.408285	2.652484	-0.356960
16	1	0	2.602247	-2.196491	-0.488823
17	1	0	1.092151	-3.671193	-0.146682
18	1	0	1.249341	-2.730918	-2.053837
19	1	0	-2.209056	-1.149426	-1.732684
20	1	0	-2.329609	-2.598746	-0.647813
21	1	0	-2.573953	1.231848	1.243068
22	1	0	-3.336170	-0.580477	2.383565
23	1	0	-3.379181	-2.256425	1.593031
24	1	0	-0.742920	1.968099	1.689910
25	1	0	1.019568	0.514770	2.014901
26	1	0	-3.623218	1.659791	-0.943452
27	1	0	-2.184579	1.088646	-1.796060
28	1	0	4.649227	1.694861	0.113946
29	1	0	4.454927	0.108155	-0.655910
30	1	0	5.153376	0.215597	0.993048
31	1	0	-1.926907	3.545341	-1.659137
32	1	0	-2.358632	3.527513	0.053801
33	1	0	0.113466	3.545640	0.010840
34	1	0	0.152744	2.299588	-1.223841

TS(3,4)Z_t´

Zero-point correction= 0.277528 (Hartree/Particle)
Thermal correction to Energy= 0.295384
Thermal correction to Enthalpy= 0.296329
Thermal correction to Gibbs Free Energy= 0.230429
Sum of electronic and zero-point Energies= -1048.791963
Sum of electronic and thermal Energies= -1048.774107
Sum of electronic and thermal Enthalpies= -1048.773162
Sum of electronic and thermal Free Energies= -1048.839062

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.072086	-0.899931	-0.021038
2	15	0	-1.493860	-2.509547	-0.012507
3	6	0	2.518798	-0.894187	-0.112916
4	6	0	1.728495	-1.910690	-0.850688
5	6	0	2.002683	0.501915	-0.391840
6	6	0	3.453193	-1.183950	0.823685
7	6	0	0.533722	1.399392	0.696680
8	6	0	-0.816718	0.843689	0.890455
9	6	0	2.938217	1.652589	-0.049835
10	6	0	-1.957563	1.232368	0.058421
11	8	0	-1.936980	1.752855	-1.049288
12	8	0	-3.140564	0.888964	0.664674
13	6	0	-4.317159	1.201751	-0.086474
14	6	0	2.214218	2.978378	-0.314900
15	6	0	0.718384	2.749771	0.006972
16	1	0	-2.363656	-2.637247	1.095580
17	1	0	-1.140613	-3.872665	-0.140536
18	1	0	-2.477215	-2.466000	-1.026864
19	1	0	1.652386	-1.755690	-1.931425
20	1	0	1.930790	-2.952080	-0.594743
21	1	0	1.662407	0.594251	-1.428578
22	1	0	3.932614	-0.423679	1.431146
23	1	0	3.758968	-2.211603	0.997797
24	1	0	1.099543	1.322570	1.626411
25	1	0	-1.077173	0.559815	1.907158
26	1	0	3.242220	1.585930	1.001522
27	1	0	3.855718	1.546276	-0.643588
28	1	0	-4.371662	2.273023	-0.301020
29	1	0	-4.336234	0.657471	-1.036134
30	1	0	-5.156825	0.897604	0.541166
31	1	0	2.332646	3.273224	-1.363855
32	1	0	2.644927	3.784902	0.288287
33	1	0	0.326201	3.521654	0.682629
34	1	0	0.099626	2.781578	-0.890070

TS(3,4)*E´*

Zero-point correction= 0.277638 (Hartree/Particle)
Thermal correction to Energy= 0.295372
Thermal correction to Enthalpy= 0.296316
Thermal correction to Gibbs Free Energy= 0.230676
Sum of electronic and zero-point Energies= -1048.792766
Sum of electronic and thermal Energies= -1048.775031
Sum of electronic and thermal Enthalpies= -1048.774087
Sum of electronic and thermal Free Energies= -1048.839727

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.078080	0.887602	-0.128985
2	15	0	-1.221264	2.573155	-0.827669
3	6	0	1.684329	0.455350	1.547577
4	6	0	1.697954	1.780936	0.895950
5	6	0	1.785369	-0.759509	0.619374

6	6	0	1.402346	0.270619	2.862996
7	6	0	0.441348	-1.543653	-0.542152
8	6	0	-0.816931	-0.861220	-0.954772
9	6	0	3.008854	-0.841361	-0.291724
10	6	0	-2.107559	-1.139886	-0.315651
11	8	0	-3.199340	-0.834154	-0.774116
12	8	0	-1.982682	-1.768219	0.894328
13	6	0	-3.213583	-2.009078	1.581553
14	6	0	2.802320	-2.060366	-1.195112
15	6	0	1.360216	-1.945827	-1.697835
16	1	0	-1.833640	2.500437	-2.099527
17	1	0	-2.382337	2.810045	-0.058917
18	1	0	-0.757222	3.907275	-0.907191
19	1	0	2.476784	1.966032	0.153867
20	1	0	1.547142	2.631242	1.561182
21	1	0	1.760815	-1.633036	1.271500
22	1	0	1.273097	-0.720964	3.287878
23	1	0	1.298278	1.115687	3.537739
24	1	0	0.224464	-2.360305	0.144113
25	1	0	-0.931482	-0.678196	-2.022306
26	1	0	3.921369	-0.926947	0.313107
27	1	0	3.107633	0.066658	-0.898911
28	1	0	-3.882632	-2.631172	0.979863
29	1	0	-3.723571	-1.067923	1.809035
30	1	0	-2.940856	-2.523899	2.504423
31	1	0	3.523803	-2.102773	-2.018670
32	1	0	2.925657	-2.980943	-0.607749
33	1	0	1.002963	-2.881341	-2.146895
34	1	0	1.305227	-1.173950	-2.477099

TS(3,4)E_t'

Zero-point correction= 0.277644 (Hartree/Particle)
Thermal correction to Energy= 0.295362
Thermal correction to Enthalpy= 0.296306
Thermal correction to Gibbs Free Energy= 0.231333
Sum of electronic and zero-point Energies= -1048.793624
Sum of electronic and thermal Energies= -1048.775906
Sum of electronic and thermal Enthalpies= -1048.774962
Sum of electronic and thermal Free Energies= -1048.839935

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.223718	-0.897566	-0.292805
2	15	0	2.208406	-1.908464	-0.570511
3	6	0	-1.799335	-1.267878	1.047944
4	6	0	-1.018907	-2.410775	0.505631
5	6	0	-2.072174	-0.237239	-0.028571
6	6	0	-2.073208	-1.078622	2.359786
7	6	0	-0.827059	1.304178	-0.441844
8	6	0	0.557199	1.138625	-0.903477
9	6	0	-3.193945	0.757227	0.239474
10	6	0	1.714693	1.617262	-0.140378
11	8	0	2.859605	1.673595	-0.569133
12	8	0	1.405820	1.979806	1.142680
13	6	0	2.515983	2.401105	1.939600
14	6	0	-3.258937	1.749376	-0.929015
15	6	0	-1.803933	1.956541	-1.415451

16	1	0	3.353902	-1.079513	-0.595726
17	1	0	2.656955	-2.887907	0.344688
18	1	0	2.435078	-2.636132	-1.760841
19	1	0	-1.463232	-2.914055	-0.359235
20	1	0	-0.641025	-3.119504	1.244110
21	1	0	-2.244463	-0.725994	-0.994589
22	1	0	-2.536594	-0.173569	2.738371
23	1	0	-1.822233	-1.841165	3.091479
24	1	0	-0.873094	1.714360	0.565938
25	1	0	0.733257	1.166812	-1.977738
26	1	0	-3.006113	1.287902	1.180103
27	1	0	-4.132011	0.203618	0.375724
28	1	0	3.019889	3.259109	1.485375
29	1	0	3.243415	1.591864	2.057254
30	1	0	2.095874	2.674146	2.909029
31	1	0	-3.877396	1.345786	-1.738883
32	1	0	-3.722226	2.691987	-0.619152
33	1	0	-1.547113	3.020530	-1.494700
34	1	0	-1.655663	1.530681	-2.415076

4Z´

Zero-point correction= 0.279877 (Hartree/Particle)
Thermal correction to Energy= 0.297872
Thermal correction to Enthalpy= 0.298816
Thermal correction to Gibbs Free Energy= 0.232841
Sum of electronic and zero-point Energies= -1048.839291
Sum of electronic and thermal Energies= -1048.821296
Sum of electronic and thermal Enthalpies= -1048.820352
Sum of electronic and thermal Free Energies= -1048.886327

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.360820	-1.268049	-0.258461
2	15	0	-2.115200	-1.508781	1.431276
3	6	0	2.389630	-0.652371	-0.728230
4	6	0	3.317679	-1.377352	-0.073255
5	6	0	2.346599	0.872370	-0.730807
6	6	0	1.298638	-1.302928	-1.486869
7	6	0	1.011141	1.416445	-0.137515
8	6	0	-0.252923	0.795915	-0.723014
9	6	0	3.382992	1.588211	0.158176
10	6	0	-1.540505	1.350208	-0.217641
11	8	0	-1.830647	1.606388	0.942615
12	8	0	-2.421403	1.553194	-1.236222
13	6	0	-3.700617	2.069305	-0.852343
14	6	0	2.754310	1.638584	1.579380
15	6	0	1.243242	1.330327	1.386854
16	1	0	-3.426689	-1.020917	1.231294
17	1	0	-2.488306	-2.802022	1.881517
18	1	0	-1.901499	-0.936238	2.703722
19	1	0	4.099518	-0.929362	0.530605
20	1	0	3.320691	-2.463291	-0.133231
21	1	0	2.439858	1.193352	-1.779160
22	1	0	1.089496	-0.846187	-2.457879
23	1	0	1.427659	-2.390385	-1.597253
24	1	0	0.986309	2.488825	-0.402681
25	1	0	-0.249339	0.860329	-1.811448

26	1	0	3.519110	2.606535	-0.225123
27	1	0	4.369536	1.116046	0.137248
28	1	0	-3.595329	3.028643	-0.337898
29	1	0	-4.220522	1.372095	-0.187603
30	1	0	-4.258664	2.192684	-1.781550
31	1	0	3.217013	0.901747	2.244505
32	1	0	2.912195	2.619762	2.040728
33	1	0	0.587530	2.007506	1.938307
34	1	0	1.012428	0.313927	1.726397

4 Z_t'

Zero-point correction= 0.279639 (Hartree/Particle)
Thermal correction to Energy= 0.297921
Thermal correction to Enthalpy= 0.298865
Thermal correction to Gibbs Free Energy= 0.231970
Sum of electronic and zero-point Energies= -1048.841130
Sum of electronic and thermal Energies= -1048.822848
Sum of electronic and thermal Enthalpies= -1048.821904
Sum of electronic and thermal Free Energies= -1048.888799

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.311168	-0.897619	0.166785
2	15	0	3.371474	-0.190640	-0.982830
3	6	0	-1.550220	-1.694033	0.774287
4	6	0	-2.081574	-2.925719	0.668236
5	6	0	-2.206324	-0.447523	0.228053
6	6	0	-0.241091	-1.444804	1.411630
7	6	0	-3.617489	-0.540401	-0.370952
8	6	0	-3.774956	0.767106	-1.188561
9	6	0	-2.328398	1.237752	-1.527424
10	6	0	-1.392964	0.133523	-0.958200
11	6	0	0.051413	0.552907	-0.731868
12	6	0	0.407189	1.761674	0.064920
13	8	0	1.408830	2.438136	-0.124827
14	8	0	-0.483072	2.060474	1.049436
15	6	0	-0.137772	3.186984	1.867001
16	1	0	4.395656	-1.068535	-1.424483
17	1	0	3.250180	0.544313	-2.183993
18	1	0	4.210954	0.721100	-0.303426
19	1	0	-3.043114	-3.108610	0.199248
20	1	0	-1.566235	-3.796048	1.068093
21	1	0	-2.216030	0.308701	1.025053
22	1	0	-0.279464	-0.625623	2.139291
23	1	0	0.194600	-2.346683	1.871160
24	1	0	-4.397437	-0.663780	0.388044
25	1	0	-3.676843	-1.406562	-1.042068
26	1	0	-4.291662	1.530582	-0.596185
27	1	0	-4.378676	0.607637	-2.088273
28	1	0	-2.171276	1.381323	-2.601964
29	1	0	-2.116362	2.194605	-1.039475
30	1	0	-1.349169	-0.676360	-1.701399
31	1	0	0.564409	0.648109	-1.691534
32	1	0	0.808105	3.010526	2.387302
33	1	0	-0.953740	3.289330	2.583797
34	1	0	-0.042696	4.092371	1.261538

4*E*´

Zero-point correction= 0.279836 (Hartree/Particle)
Thermal correction to Energy= 0.297974
Thermal correction to Enthalpy= 0.298918
Thermal correction to Gibbs Free Energy= 0.231834
Sum of electronic and zero-point Energies= -1048.850185
Sum of electronic and thermal Energies= -1048.832047
Sum of electronic and thermal Enthalpies= -1048.831103
Sum of electronic and thermal Free Energies= -1048.898187

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.162610	-0.201463	-0.275770
2	15	0	3.396935	-0.985653	-0.191162
3	6	0	-0.916742	-1.973670	0.931774
4	6	0	0.263170	-2.053215	0.032527
5	6	0	-2.143651	-1.197396	0.495361
6	6	0	-0.906117	-2.573937	2.136675
7	6	0	-2.771063	-1.579369	-0.869442
8	6	0	-3.636273	-0.352706	-1.280366
9	6	0	-3.289579	0.773878	-0.266598
10	6	0	-1.950714	0.343905	0.382255
11	6	0	-0.743284	0.729892	-0.450231
12	6	0	-0.025007	1.974614	-0.174659
13	8	0	1.104083	2.179538	-0.671638
14	8	0	-0.566368	2.824349	0.716383
15	6	0	0.259652	3.928107	1.120204
16	1	0	3.652953	-2.339287	0.137254
17	1	0	4.230976	-0.925856	-1.335155
18	1	0	4.322695	-0.412342	0.715349
19	1	0	0.007046	-2.348249	-0.991306
20	1	0	1.014449	-2.743164	0.426245
21	1	0	-2.916757	-1.351347	1.260809
22	1	0	-1.759890	-2.527689	2.808489
23	1	0	-0.041683	-3.132057	2.489811
24	1	0	-3.352258	-2.505029	-0.799217
25	1	0	-1.988474	-1.755235	-1.615465
26	1	0	-4.706415	-0.584976	-1.257713
27	1	0	-3.408815	-0.045653	-2.307251
28	1	0	-3.230097	1.763597	-0.731795
29	1	0	-4.062587	0.830945	0.510385
30	1	0	-1.839122	0.776737	1.381339
31	1	0	-0.858624	0.587359	-1.529055
32	1	0	0.506592	4.560594	0.263656
33	1	0	1.185973	3.568207	1.576649
34	1	0	-0.334122	4.483844	1.846867

4*E*$_t$´

Zero-point correction= 0.279446 (Hartree/Particle)
Thermal correction to Energy= 0.297707
Thermal correction to Enthalpy= 0.298652
Thermal correction to Gibbs Free Energy= 0.231572
Sum of electronic and zero-point Energies= -1048.841093
Sum of electronic and thermal Energies= -1048.822831
Sum of electronic and thermal Enthalpies= -1048.821887
Sum of electronic and thermal Free Energies= -1048.888966

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.975628	-1.192863	-0.088458
2	15	0	-3.358356	-0.533384	0.077830
3	6	0	1.993725	-1.705621	0.281498
4	6	0	2.580921	-2.302629	1.334300
5	6	0	2.474216	-0.410763	-0.328527
6	6	0	0.778430	-2.240239	-0.362678
7	6	0	3.810063	0.194182	0.127783
8	6	0	3.754604	1.665960	-0.359437
9	6	0	2.246308	1.985505	-0.578071
10	6	0	1.475620	0.740885	-0.056981
11	6	0	0.091728	0.567617	-0.658046
12	6	0	-0.897698	1.633969	-0.329336
13	8	0	-1.879692	1.923420	-0.999340
14	8	0	-0.617482	2.278951	0.835535
15	6	0	-1.536250	3.313386	1.204285
16	1	0	-4.292765	-1.513899	0.503146
17	1	0	-3.840533	0.511565	0.899438
18	1	0	-4.026894	-0.157353	-1.106674
19	1	0	3.474616	-1.907335	1.806859
20	1	0	2.183545	-3.225338	1.750664
21	1	0	2.518967	-0.552824	-1.422359
22	1	0	0.875086	-2.307371	-1.453379
23	1	0	0.459359	-3.210747	0.050404
24	1	0	4.678067	-0.351247	-0.257385
25	1	0	3.869778	0.168150	1.222647
26	1	0	4.311883	1.787591	-1.294943
27	1	0	4.214609	2.343382	0.367753
28	1	0	1.923926	2.897487	-0.067664
29	1	0	2.036816	2.124632	-1.646738
30	1	0	1.378409	0.827074	1.032302
31	1	0	0.114452	0.445136	-1.744968
32	1	0	-1.607813	4.069813	0.417962
33	1	0	-1.135538	3.748695	2.120795
34	1	0	-2.534368	2.902558	1.385477

4*Z*

Zero-point correction= 0.308043 (Hartree/Particle)
Thermal correction to Energy= 0.329311
Thermal correction to Enthalpy= 0.330255
Thermal correction to Gibbs Free Energy= 0.256782
Sum of electronic and zero-point Energies= -1391.971460
Sum of electronic and thermal Energies= -1391.950192
Sum of electronic and thermal Enthalpies= -1391.949248
Sum of electronic and thermal Free Energies= -1392.022721

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.284614	1.010517	-0.162755
2	15	0	1.975918	0.835859	1.595306
3	6	0	-2.426811	0.175440	-0.736380
4	6	0	-3.443554	0.787942	-0.100079
5	6	0	-2.253205	-1.339885	-0.777526

6	6	0	-1.396127	0.964666	-1.463252
7	6	0	-0.893940	-1.810425	-0.181335
8	6	0	0.330408	-1.071431	-0.723906
9	6	0	-3.247067	-2.162327	0.068026
10	6	0	1.629760	-1.656305	-0.317015
11	8	0	1.934614	-2.100475	0.783970
12	8	0	2.531184	-1.646016	-1.345008
13	6	0	3.820153	-2.185757	-1.041081
14	6	0	-2.644638	-2.202115	1.500313
15	6	0	-1.156454	-1.783218	1.340343
16	15	0	0.028294	3.383320	-0.016324
17	1	0	3.272697	0.322277	1.373233
18	1	0	2.371954	2.009031	2.290797
19	1	0	1.652611	0.055215	2.724200
20	1	0	-4.196181	0.251495	0.467067
21	1	0	-3.552352	1.870248	-0.132773
22	1	0	-2.307755	-1.633841	-1.836801
23	1	0	-1.069047	0.506901	-2.399731
24	1	0	-1.737470	1.984421	-1.667173
25	1	0	-0.798263	-2.872311	-0.469301
26	1	0	0.305733	-1.046111	-1.814616
27	1	0	-3.286577	-3.177086	-0.346048
28	1	0	-4.270393	-1.776878	0.037634
29	1	0	3.741427	-3.225837	-0.711272
30	1	0	4.315805	-1.609410	-0.253047
31	1	0	4.391984	-2.122716	-1.968453
32	1	0	-3.171182	-1.514494	2.171113
33	1	0	-2.741466	-3.202173	1.937782
34	1	0	-0.460563	-2.426789	1.883230
35	1	0	-1.007769	-0.760834	1.709317
36	1	0	0.327192	4.119287	-1.188277
37	1	0	-1.271846	3.906464	0.182504
38	1	0	0.698473	4.244116	0.892276

4 Z_t

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Zero-point correction=                           0.307757 (Hartree/Particle)
 Thermal correction to Energy=                    0.329331
 Thermal correction to Enthalpy=                  0.330275
 Thermal correction to Gibbs Free Energy=         0.255875
 Sum of electronic and zero-point Energies=          -1391.976340
 Sum of electronic and thermal Energies=             -1391.954766
 Sum of electronic and thermal Enthalpies=           -1391.953822
 Sum of electronic and thermal Free Energies=        -1392.028222
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.146354	-0.371979	0.108942
2	15	0	-2.779970	-2.025972	-0.424160
3	15	0	-2.550163	1.001240	1.558336
4	1	0	-4.099112	-2.103944	0.094487
5	1	0	-3.120613	-2.223094	-1.783852
6	1	0	-2.407675	-3.361537	-0.143337
7	1	0	-3.365969	1.959375	0.910506
8	1	0	-3.556686	0.494372	2.422808
9	1	0	-1.955455	1.883203	2.491163
10	6	0	1.365429	-1.866863	-0.688980
11	6	0	1.567883	-3.188460	-0.533794

12	6	0	2.367482	-0.814787	-0.279690
13	6	0	0.128893	-1.330114	-1.309784
14	6	0	3.712724	-1.255893	0.318669
15	6	0	4.278200	0.022568	0.999102
16	6	0	3.068389	0.987775	1.165212
17	6	0	1.822131	0.137618	0.812947
18	6	0	0.547701	0.918140	0.513900
19	6	0	0.568279	1.866655	-0.619749
20	8	0	1.262801	1.820753	-1.624341
21	8	0	-0.353648	2.874687	-0.442444
22	6	0	-0.447428	3.806290	-1.523246
23	1	0	2.475359	-3.593625	-0.097933
24	1	0	0.826219	-3.914216	-0.862408
25	1	0	2.567162	-0.194864	-1.164613
26	1	0	-0.431073	-2.114542	-1.829879
27	1	0	0.328382	-0.505370	-2.000182
28	1	0	4.393770	-1.673967	-0.430440
29	1	0	3.544246	-2.035192	1.072976
30	1	0	5.057611	0.483587	0.382572
31	1	0	4.742475	-0.216764	1.962131
32	1	0	3.002806	1.417788	2.171387
33	1	0	3.147340	1.821401	0.458347
34	1	0	1.596364	-0.498039	1.683878
35	1	0	0.230121	1.452315	1.412270
36	1	0	-0.769734	3.308445	-2.443520
37	1	0	0.516029	4.289635	-1.709505
38	1	0	-1.188592	4.545970	-1.214079

4*E*

Zero-point correction= 0.308008 (Hartree/Particle)
Thermal correction to Energy= 0.329233
Thermal correction to Enthalpy= 0.330178
Thermal correction to Gibbs Free Energy= 0.256675
Sum of electronic and zero-point Energies= -1391.975076
Sum of electronic and thermal Energies= -1391.953851
Sum of electronic and thermal Enthalpies= -1391.952907
Sum of electronic and thermal Free Energies= -1392.026409

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.107231	-0.113965	-0.024997
2	15	0	-1.831386	1.461567	1.728006
3	6	0	0.567272	-2.380429	-0.610417
4	6	0	0.223024	-3.617186	-0.201346
5	6	0	1.936292	-1.794766	-0.312438
6	6	0	-0.350796	-1.528292	-1.402070
7	6	0	2.516229	-2.068971	1.099308
8	6	0	3.552925	-0.936521	1.351708
9	6	0	3.450659	0.010506	0.126989
10	6	0	2.052511	-0.258876	-0.484691
11	6	0	0.949096	0.525077	0.226958
12	15	0	-3.284209	-0.943469	-0.528727
13	6	0	0.877988	1.972135	-0.088061
14	8	0	0.411263	2.841294	0.645279
15	8	0	1.374216	2.291320	-1.315046
16	6	0	1.277479	3.671663	-1.679100
17	1	0	-2.197470	2.784759	1.405451
18	1	0	-3.008911	1.126621	2.453271

19	1	0	-1.014972	1.735049	2.844166
20	1	0	0.886231	-4.234193	0.397992
21	1	0	-0.737278	-4.054941	-0.466368
22	1	0	2.635879	-2.232321	-1.042692
23	1	0	0.141210	-0.932928	-2.174569
24	1	0	-1.161199	-2.108606	-1.855348
25	1	0	2.963999	-3.065881	1.169341
26	1	0	1.710225	-2.035029	1.841162
27	1	0	4.569841	-1.326824	1.468390
28	1	0	3.318472	-0.402217	2.279233
29	1	0	3.603790	1.063213	0.388340
30	1	0	4.220163	-0.250016	-0.611847
31	1	0	2.050009	0.009396	-1.544066
32	1	0	1.031368	0.429080	1.314146
33	1	0	-3.703685	-0.903856	-1.880061
34	1	0	-3.519127	-2.323415	-0.318929
35	1	0	-4.498308	-0.476633	0.038522
36	1	0	1.815980	4.302864	-0.966528
37	1	0	0.232227	3.993961	-1.711574
38	1	0	1.728199	3.745896	-2.670251

4 E_t

Zero-point correction= 0.307625 (Hartree/Particle)
Thermal correction to Energy= 0.329053
Thermal correction to Enthalpy= 0.329998
Thermal correction to Gibbs Free Energy= 0.255875
Sum of electronic and zero-point Energies= -1391.971615
Sum of electronic and thermal Energies= -1391.950187
Sum of electronic and thermal Enthalpies= -1391.949242
Sum of electronic and thermal Free Energies= -1392.023365

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.186939	-0.374750	-0.177776
2	15	0	-2.532079	1.642881	0.193624
3	6	0	1.113577	-2.345986	0.006987
4	6	0	1.227517	-3.326940	0.920507
5	6	0	2.226591	-1.385923	-0.329713
6	6	0	-0.130921	-2.129348	-0.768099
7	6	0	3.610715	-1.594597	0.301967
8	6	0	4.357073	-0.259982	0.038363
9	6	0	3.249711	0.791751	-0.262754
10	6	0	1.902098	0.081433	0.039851
11	6	0	0.674675	0.665526	-0.659667
12	6	0	0.446725	2.112885	-0.422392
13	8	0	-0.144274	2.885437	-1.167619
14	8	0	0.949802	2.548549	0.774060
15	6	0	0.823424	3.951213	1.023026
16	1	0	-3.801988	1.503828	0.814219
17	1	0	-2.108093	2.769876	0.931125
18	1	0	-2.970533	2.320513	-0.963269
19	1	0	2.138739	-3.498643	1.484101
20	1	0	0.400533	-4.003992	1.125892
21	1	0	2.353133	-1.414129	-1.426667
22	1	0	0.062343	-1.919561	-1.825585
23	1	0	-0.794917	-2.997632	-0.703045
24	1	0	4.135740	-2.466484	-0.103023

25	1	0	3.501711	-1.754468	1.381843
26	1	0	5.041491	-0.356206	-0.812066
27	1	0	4.969749	0.027727	0.899639
28	1	0	3.364440	1.707347	0.322495
29	1	0	3.275477	1.081047	-1.321990
30	1	0	1.740544	0.109146	1.126358
31	1	0	0.717962	0.524600	-1.744707
32	1	0	1.321370	4.532754	0.241628
33	1	0	1.302069	4.122588	1.988825
34	1	0	-0.226476	4.257512	1.063318
35	15	0	-2.991101	-1.849798	0.340966
36	1	0	-4.277071	-1.468760	0.806288
37	1	0	-3.429963	-2.758418	-0.651875
38	1	0	-2.720729	-2.808486	1.345347

TS(4,5)*Z*

Zero-point correction= 0.305217 (Hartree/Particle)
Thermal correction to Energy= 0.327013
Thermal correction to Enthalpy= 0.327957
Thermal correction to Gibbs Free Energy= 0.251703
Sum of electronic and zero-point Energies= -1391.927361
Sum of electronic and thermal Energies= -1391.905565
Sum of electronic and thermal Enthalpies= -1391.904621
Sum of electronic and thermal Free Energies= -1391.980875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.087283	-0.651166	0.193346
2	15	0	-1.171465	-0.262210	2.522255
3	15	0	-3.124383	-1.079796	-1.053485
4	1	0	-1.561311	-1.299796	3.411732
5	1	0	-0.075706	0.168071	3.322524
6	1	0	-2.077179	0.694129	3.056134
7	1	0	-3.148478	-1.185699	-2.471086
8	1	0	-3.965981	-2.206523	-0.838356
9	1	0	-4.174558	-0.129789	-0.986808
10	6	0	2.065667	-1.574782	-0.501137
11	6	0	2.549341	-2.479969	0.361548
12	6	0	2.840303	-0.410304	-1.084194
13	6	0	0.651984	-1.600056	-0.946494
14	6	0	4.175422	-0.053381	-0.416107
15	6	0	3.793237	0.778790	0.839461
16	6	0	2.303195	1.183920	0.655184
17	6	0	1.952484	0.830724	-0.809650
18	6	0	0.504104	0.529174	-1.181974
19	1	0	3.582201	-2.471897	0.696280
20	1	0	1.921267	-3.274559	0.757085
21	1	0	2.955787	-0.574995	-2.166189
22	1	0	0.078961	-2.393609	-0.439249
23	1	0	0.529670	-1.710428	-2.023540
24	1	0	4.761555	0.558389	-1.112359
25	1	0	4.789788	-0.928715	-0.182332
26	1	0	4.440938	1.657306	0.933754
27	1	0	3.923526	0.195443	1.756881
28	1	0	1.661986	0.604765	1.326022
29	1	0	2.122717	2.237854	0.872609
30	1	0	2.293161	1.653023	-1.459181

31	1	0	0.417985	0.329106	-2.247248
32	6	0	-0.538346	1.587926	-0.931595
33	8	0	-1.471702	1.815665	-1.689332
34	8	0	-0.284822	2.386113	0.145864
35	6	0	-1.230122	3.444136	0.346725
36	1	0	-2.222637	3.037612	0.562682
37	1	0	-1.295492	4.081876	-0.538885
38	1	0	-0.856892	4.010873	1.201198

TS(4,5) Z_t

Zero-point correction= 0.304821 (Hartree/Particle)
Thermal correction to Energy= 0.326925
Thermal correction to Enthalpy= 0.327869
Thermal correction to Gibbs Free Energy= 0.249839
Sum of electronic and zero-point Energies= -1391.933244
Sum of electronic and thermal Energies= -1391.911139
Sum of electronic and thermal Enthalpies= -1391.910195
Sum of electronic and thermal Free Energies= -1391.988225

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.421657	-0.577919	-0.053790
2	15	0	1.550984	-2.781225	-0.924429
3	15	0	3.332513	0.823348	0.193490
4	1	0	2.178145	-3.804961	-0.164704
5	1	0	0.426158	-3.579876	-1.277734
6	1	0	2.269550	-3.066170	-2.116949
7	1	0	3.359225	1.970013	1.035559
8	1	0	4.617013	0.362759	0.593532
9	1	0	3.807280	1.511392	-0.954000
10	6	0	-1.513460	-1.147806	1.403203
11	6	0	-1.619615	-2.387184	1.905426
12	6	0	-2.564820	-0.409892	0.629710
13	6	0	-0.278198	-0.334193	1.496807
14	6	0	-3.870071	-1.045163	0.145821
15	6	0	-4.271704	-0.167363	-1.085541
16	6	0	-3.011106	0.675612	-1.465963
17	6	0	-1.871293	-0.008793	-0.685999
18	6	0	-0.541156	0.686098	-0.453074
19	6	0	-0.575012	2.083430	0.050007
20	8	0	-1.408873	2.557178	0.806447
21	8	0	0.459397	2.827358	-0.431377
22	6	0	0.495301	4.186246	0.024567
23	1	0	-2.545875	-2.951545	1.842565
24	1	0	-0.788974	-2.867536	2.417365
25	1	0	-2.795189	0.521178	1.166871
26	1	0	0.564018	-0.852622	1.981474
27	1	0	-0.436510	0.635235	1.962964
28	1	0	-4.650590	-1.068391	0.913253
29	1	0	-3.689517	-2.081330	-0.167944
30	1	0	-5.114577	0.488526	-0.843887
31	1	0	-4.595083	-0.797061	-1.921130
32	1	0	-2.833554	0.700941	-2.546576
33	1	0	-3.124009	1.709282	-1.122278
34	1	0	-1.625668	-0.948022	-1.204231
35	1	0	0.108618	0.629762	-1.338428
36	1	0	0.586857	4.228224	1.113819
37	1	0	-0.413438	4.718113	-0.270975

38	1	0	1.370069	4.632265	-0.450506

TS(4,5)*E*

Zero-point correction= 0.304824 (Hartree/Particle)
Thermal correction to Energy= 0.326682
Thermal correction to Enthalpy= 0.327626
Thermal correction to Gibbs Free Energy= 0.250963
Sum of electronic and zero-point Energies= -1391.936419
Sum of electronic and thermal Energies= -1391.914561
Sum of electronic and thermal Enthalpies= -1391.913617
Sum of electronic and thermal Free Energies= -1391.990280

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.932020	-0.963269	0.043174
2	15	0	3.302544	-0.583208	0.010898
3	15	0	0.143185	-3.168939	-0.419136
4	1	0	3.918333	0.465307	0.747597
5	1	0	4.274952	-1.558907	0.364721
6	1	0	3.921145	-0.242194	-1.220583
7	1	0	0.657330	-4.318880	0.240438
8	1	0	-1.217918	-3.566617	-0.290569
9	1	0	0.303327	-3.706200	-1.724721
10	6	0	-1.935184	-0.067203	1.353290
11	6	0	-2.604053	-1.105557	1.877038
12	6	0	-2.537305	1.070353	0.556495
13	6	0	-0.473325	0.086718	1.495100
14	6	0	-1.659933	1.194192	-0.716044
15	6	0	-0.159930	1.020512	-0.474715
16	6	0	-3.955876	0.875472	-0.002962
17	6	0	-3.783073	0.090545	-1.335229
18	6	0	-2.266582	0.136640	-1.664211
19	6	0	0.536092	2.258879	-0.034232
20	8	0	0.066081	3.108095	0.705162
21	8	0	1.788086	2.375632	-0.559796
22	6	0	2.501858	3.556397	-0.169332
23	1	0	-3.680464	-1.211810	1.781311
24	1	0	-2.090845	-1.880794	2.440976
25	1	0	-2.455359	1.984744	1.157446
26	1	0	-0.182457	1.051612	1.903740
27	1	0	0.008027	-0.722520	2.065743
28	1	0	-1.823714	2.193673	-1.144333
29	1	0	0.330718	0.619134	-1.374903
30	1	0	-4.390833	1.861838	-0.202485
31	1	0	-4.632006	0.378149	0.699869
32	1	0	-4.127291	-0.944196	-1.237403
33	1	0	-4.381233	0.544701	-2.132634
34	1	0	-2.065708	0.368530	-2.716264
35	1	0	-1.801688	-0.834157	-1.455507
36	1	0	2.646422	3.582440	0.914666
37	1	0	1.957763	4.455575	-0.471574
38	1	0	3.463155	3.501620	-0.682094

TS(4,5)E_t

Zero-point correction= 0.304778 (Hartree/Particle)

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 Thermal correction to Energy=                  0.326712
 Thermal correction to Enthalpy=                0.327656
 Thermal correction to Gibbs Free Energy=       0.250692
 Sum of electronic and zero-point Energies=         -1391.931981
 Sum of electronic and thermal Energies=            -1391.910047
 Sum of electronic and thermal Enthalpies=          -1391.909103
 Sum of electronic and thermal Free Energies=       -1391.986067

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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         46             0        1.105051   -0.814553   -0.033851
    2         15             0        3.284384    0.085789   -0.427100
    3         15             0        0.882713   -3.139227   -0.516423
    4          1             0        3.838883    1.094645    0.405912
    5          1             0        4.465250   -0.705820   -0.454364
    6          1             0        3.563839    0.762528   -1.643315
    7          1             0        1.901829   -4.092755   -0.245319
    8          1             0       -0.174407   -3.939130   -0.001065
    9          1             0        0.704971   -3.543450   -1.866959
   10          6             0       -1.848235   -1.086684    1.095985
   11          6             0       -2.359839   -2.128928    1.762932
   12          6             0       -2.464320   -0.440028   -0.121194
   13          6             0       -0.570841   -0.402927    1.462105
   14          6             0       -1.929435    0.993081   -0.178875
   15          6             0       -0.404812    0.977638   -0.155420
   16          6             0       -3.976703   -0.267653   -0.309869
   17          6             0       -4.091980    0.933024   -1.306509
   18          6             0       -2.670225    1.575126   -1.396156
   19          6             0        0.212240    2.196115    0.442468
   20          8             0       -0.179077    2.750926    1.455018
   21          8             0        1.268039    2.667664   -0.278070
   22          6             0        1.879696    3.852832    0.250502
   23          1             0       -3.303300   -2.582708    1.469696
   24          1             0       -1.865333   -2.553861    2.633026
   25          1             0       -2.059823   -0.965463   -1.004832
   26          1             0       -0.711726    0.517160    2.029242
   27          1             0        0.145070   -1.028221    2.019080
   28          1             0       -2.276353    1.521865    0.719134
   29          1             0       -0.007305    0.779956   -1.161738
   30          1             0       -4.441143   -0.018569    0.651700
   31          1             0       -4.471577   -1.169815   -0.684364
   32          1             0       -4.431729    0.603142   -2.293956
   33          1             0       -4.830117    1.658841   -0.949579
   34          1             0       -2.701429    2.669607   -1.397828
   35          1             0       -2.167906    1.262054   -2.321121
   36          1             0        2.291300    3.666609    1.246744
   37          1             0        1.151911    4.666097    0.318578
   38          1             0        2.675310    4.110003   -0.450060
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TS(4,5)*Z´*

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Zero-point correction=                          0.278839 (Hartree/Particle)
 Thermal correction to Energy=                  0.296704
 Thermal correction to Enthalpy=                0.297648
 Thermal correction to Gibbs Free Energy=       0.230492
 Sum of electronic and zero-point Energies=         -1048.809874
 Sum of electronic and thermal Energies=            -1048.792009
 Sum of electronic and thermal Enthalpies=          -1048.791065
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Sum of electronic and thermal Free Energies= -1048.858221

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.916493	-0.965019	-0.177558
2	15	0	-2.756825	-1.336233	1.140845
3	1	0	-3.314218	-2.633975	1.276347
4	1	0	-2.736565	-1.043462	2.528391
5	1	0	-3.984221	-0.681204	0.868574
6	6	0	2.221589	-1.101041	-0.641064
7	6	0	2.772683	-2.179273	-0.069747
8	6	0	2.785261	0.308997	-0.594070
9	6	0	0.923846	-1.170391	-1.371409
10	6	0	3.794020	0.611686	0.522558
11	6	0	2.930995	0.812041	1.795943
12	6	0	1.487104	1.111426	1.298235
13	6	0	1.579737	1.219416	-0.244690
14	6	0	0.378607	0.800368	-1.082883
15	6	0	-0.949298	1.501699	-0.895540
16	8	0	-1.788587	1.616391	-1.773725
17	8	0	-1.055585	2.154003	0.299362
18	6	0	-2.268800	2.894315	0.472728
19	1	0	3.716233	-2.133130	0.465601
20	1	0	2.297995	-3.155519	-0.127770
21	1	0	3.185827	0.559735	-1.588216
22	1	0	0.425890	-2.159280	-1.239226
23	1	0	1.000659	-1.002458	-2.444778
24	1	0	4.321868	1.539991	0.271719
25	1	0	4.561692	-0.159919	0.640298
26	1	0	3.326661	1.624272	2.415229
27	1	0	2.941108	-0.089750	2.416675
28	1	0	0.806912	0.291827	1.561477
29	1	0	1.068344	2.019236	1.736080
30	1	0	1.830566	2.256440	-0.514206
31	1	0	0.584589	0.940180	-2.141687
32	1	0	-3.133230	2.222789	0.475791
33	1	0	-2.397665	3.626426	-0.328916
34	1	0	-2.172475	3.393587	1.438181

TS(4,5)Z_t'

Zero-point correction= 0.278594 (Hartree/Particle)
Thermal correction to Energy= 0.296747
Thermal correction to Enthalpy= 0.297692
Thermal correction to Gibbs Free Energy= 0.228055
Sum of electronic and zero-point Energies= -1048.813606
Sum of electronic and thermal Energies= -1048.795453
Sum of electronic and thermal Enthalpies= -1048.794509
Sum of electronic and thermal Free Energies= -1048.864145

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.631240	-0.410504	-0.067184
2	15	0	-3.692826	-0.816376	0.844914
3	6	0	1.183544	-1.453384	-1.248961
4	6	0	1.088269	-2.708030	-1.707247

5	6	0	2.301594	-0.877824	-0.432436
6	6	0	0.120177	-0.424091	-1.432041
7	6	0	3.428338	-1.704038	0.190654
8	6	0	3.882190	-0.838572	1.414311
9	6	0	2.775282	0.244095	1.638993
10	6	0	1.596433	-0.277917	0.797338
11	6	0	0.431136	0.608111	0.390529
12	6	0	0.736058	1.953222	-0.173971
13	8	0	1.763554	2.273468	-0.748641
14	8	0	-0.288402	2.820718	0.018238
15	6	0	-0.090990	4.133916	-0.523144
16	1	0	-4.696209	-1.515917	0.124980
17	1	0	-3.830302	-1.567862	2.040115
18	1	0	-4.530948	0.253772	1.249695
19	1	0	1.893243	-3.425393	-1.572667
20	1	0	0.209734	-3.053968	-2.246142
21	1	0	2.738498	-0.036594	-0.990228
22	1	0	-0.791624	-0.822682	-1.934940
23	1	0	0.460023	0.445206	-1.992591
24	1	0	4.250534	-1.908051	-0.502858
25	1	0	3.039698	-2.672212	0.530983
26	1	0	4.850674	-0.364149	1.224968
27	1	0	4.009410	-1.464879	2.303568
28	1	0	2.521899	0.368972	2.697305
29	1	0	3.104288	1.215238	1.256317
30	1	0	1.146690	-1.123524	1.339458
31	1	0	-0.298181	0.726515	1.207526
32	1	0	0.063670	4.086977	-1.604872
33	1	0	0.777225	4.614993	-0.063963
34	1	0	-1.002307	4.685971	-0.290800

TS(4,5)*E´*

Zero-point correction= 0.278460 (Hartree/Particle)
Thermal correction to Energy= 0.296515
Thermal correction to Enthalpy= 0.297459
Thermal correction to Gibbs Free Energy= 0.228866
Sum of electronic and zero-point Energies= -1048.819136
Sum of electronic and thermal Energies= -1048.801081
Sum of electronic and thermal Enthalpies= -1048.800136
Sum of electronic and thermal Free Energies= -1048.868729

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.280794	-0.685556	0.223756
2	15	0	3.113490	-1.853496	-0.536121
3	1	0	3.834740	-2.727586	0.318117
4	1	0	3.006153	-2.768823	-1.614135
5	1	0	4.252377	-1.172669	-1.035927
6	6	0	-1.664275	-0.628196	1.321130
7	6	0	-1.937152	-1.784812	1.940046
8	6	0	-2.585141	0.127892	0.387037
9	6	0	-0.359970	0.064533	1.465290
10	6	0	-1.716587	0.459152	-0.854859
11	6	0	-0.285787	0.852785	-0.507572
12	6	0	-3.780420	-0.636397	-0.203195
13	6	0	-3.212865	-1.437168	-1.408142
14	6	0	-1.820273	-0.821257	-1.716641

15	6	0	-0.086159	2.285607	-0.147346
16	8	0	-0.945840	3.026840	0.297170
17	8	0	1.188083	2.694780	-0.368833
18	6	0	1.464058	4.056814	-0.015999
19	1	0	-2.894897	-2.285861	1.834587
20	1	0	-1.209115	-2.264456	2.589245
21	1	0	-2.893502	1.055826	0.885532
22	1	0	-0.449072	1.080780	1.845444
23	1	0	0.360527	-0.486177	2.112483
24	1	0	-2.183475	1.298258	-1.387812
25	1	0	0.408541	0.591167	-1.321790
26	1	0	-4.521188	0.093255	-0.551372
27	1	0	-4.292376	-1.271087	0.527335
28	1	0	-3.117133	-2.500513	-1.166164
29	1	0	-3.884840	-1.371383	-2.270567
30	1	0	-1.679007	-0.603733	-2.781198
31	1	0	-1.021657	-1.514869	-1.424149
32	1	0	1.271253	4.227654	1.047028
33	1	0	0.843348	4.741824	-0.600601
34	1	0	2.519945	4.209699	-0.242206

TS(4,5)E_t'

Zero-point correction= 0.278370 (Hartree/Particle)
Thermal correction to Energy= 0.296517
Thermal correction to Enthalpy= 0.297461
Thermal correction to Gibbs Free Energy= 0.228706
Sum of electronic and zero-point Energies= -1048.812747
Sum of electronic and thermal Energies= -1048.794600
Sum of electronic and thermal Enthalpies= -1048.793656
Sum of electronic and thermal Free Energies= -1048.862411

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.340863	-0.725329	0.050024
2	15	0	3.319296	-1.359881	-0.937192
3	6	0	-1.499624	-1.501389	0.990067
4	6	0	-1.794399	-2.653723	1.602594
5	6	0	-2.229195	-0.928008	-0.201927
6	6	0	-0.376315	-0.599920	1.405849
7	6	0	-1.925398	0.571921	-0.221148
8	6	0	-0.418229	0.768079	-0.183073
9	6	0	-3.751832	-0.984673	-0.377094
10	6	0	-4.054293	0.208560	-1.344762
11	6	0	-2.746240	1.060719	-1.426782
12	6	0	0.046872	2.050978	0.428361
13	8	0	-0.456924	2.580871	1.402909
14	8	0	1.100414	2.587228	-0.235355
15	6	0	1.615565	3.805311	0.319410
16	1	0	4.030112	-2.496033	-0.471366
17	1	0	3.385638	-1.707102	-2.310763
18	1	0	4.437364	-0.487872	-0.953503
19	1	0	-2.633650	-3.266622	1.283494
20	1	0	-1.218447	-3.019618	2.448844
21	1	0	-1.761195	-1.358873	-1.104503
22	1	0	-0.686244	0.250521	2.013545
23	1	0	0.435931	-1.119102	1.959791
24	1	0	-2.350467	1.021559	0.686417

25	1	0	0.020590	0.622801	-1.180058
26	1	0	-4.241005	-0.831484	0.592276
27	1	0	-4.106615	-1.942182	-0.772030
28	1	0	-4.349301	-0.146028	-2.337903
29	1	0	-4.889633	0.806910	-0.966479
30	1	0	-2.942726	2.137509	-1.405006
31	1	0	-2.206572	0.846012	-2.358624
32	1	0	1.978104	3.641197	1.338317
33	1	0	0.843068	4.579066	0.339917
34	1	0	2.436529	4.100753	-0.334982

5*Z*

Zero-point correction= 0.254330 (Hartree/Particle)
Thermal correction to Energy= 0.266692
Thermal correction to Enthalpy= 0.267637
Thermal correction to Gibbs Free Energy= 0.214789
Sum of electronic and zero-point Energies= -578.977803
Sum of electronic and thermal Energies= -578.965440
Sum of electronic and thermal Enthalpies= -578.964496
Sum of electronic and thermal Free Energies= -579.017344

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.249421	1.577038	0.029099
2	6	0	1.698416	2.483453	-0.839518
3	6	0	1.833850	0.198636	0.280075
4	6	0	0.040225	1.742098	0.927934
5	6	0	2.123566	-0.700457	-0.941608
6	6	0	1.955718	-2.121199	-0.376627
7	6	0	0.705436	-2.016273	0.525948
8	6	0	0.759556	-0.580507	1.115907
9	6	0	-0.529086	0.302922	1.097615
10	6	0	-1.481424	0.007584	-0.044651
11	8	0	-1.178280	-0.115817	-1.214487
12	8	0	-2.760974	-0.068276	0.392627
13	6	0	-3.746739	-0.293996	-0.627434
14	1	0	2.576504	2.301369	-1.454109
15	1	0	1.202589	3.441734	-0.974928
16	1	0	2.755390	0.289816	0.872412
17	1	0	-0.690407	2.465115	0.549573
18	1	0	0.358411	2.094807	1.920301
19	1	0	3.114857	-0.524024	-1.374021
20	1	0	1.372912	-0.512001	-1.715554
21	1	0	2.834425	-2.391185	0.225502
22	1	0	1.849532	-2.883985	-1.156271
23	1	0	-0.190157	-2.154965	-0.086658
24	1	0	0.686241	-2.783924	1.307105
25	1	0	1.078045	-0.626147	2.163595
26	1	0	-1.092182	0.209343	2.029396
27	1	0	-3.558907	-1.240694	-1.141324
28	1	0	-3.731874	0.514922	-1.362949
29	1	0	-4.704987	-0.323224	-0.107635

5Z_t

Zero-point correction= 0.254005 (Hartree/Particle)

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 Thermal correction to Energy=                  0.266654
 Thermal correction to Enthalpy=                0.267598
 Thermal correction to Gibbs Free Energy=       0.214072
 Sum of electronic and zero-point Energies=          -578.969391
 Sum of electronic and thermal Energies=             -578.956743
 Sum of electronic and thermal Enthalpies=           -578.955798
 Sum of electronic and thermal Free Energies=        -579.009324

 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.740989   -1.325294    0.081171
    2          6             0       -2.914200   -1.952901    0.153865
    3          6             0       -1.431946    0.109198    0.409094
    4          6             0       -0.429599   -1.915653   -0.451903
    5          6             0       -2.415817    1.278392    0.456771
    6          6             0       -1.510166    2.516458    0.118071
    7          6             0       -0.146755    1.956193   -0.419551
    8          6             0       -0.493044    0.500768   -0.740078
    9          6             0        0.484619   -0.702427   -0.847169
   10          6             0        1.660598   -0.532538    0.095131
   11          8             0        1.680285   -0.833292    1.271848
   12          8             0        2.706336    0.052216   -0.533778
   13          6             0        3.853829    0.312617    0.289831
   14          1             0       -3.800487   -1.458305    0.543203
   15          1             0       -3.034570   -2.986325   -0.163894
   16          1             0       -0.826739    0.118002    1.331466
   17          1             0       -0.605005   -2.574901   -1.308576
   18          1             0        0.063078   -2.510932    0.324901
   19          1             0       -2.921386    1.386848    1.421594
   20          1             0       -3.192360    1.147772   -0.307052
   21          1             0       -1.347863    3.143050    1.001224
   22          1             0       -1.994055    3.152530   -0.630645
   23          1             0        0.229333    2.521834   -1.278020
   24          1             0        0.618055    2.004813    0.365384
   25          1             0       -1.091268    0.487322   -1.664351
   26          1             0        0.881739   -0.796867   -1.861109
   27          1             0        4.244367   -0.618017    0.710330
   28          1             0        3.595571    0.988852    1.109452
   29          1             0        4.589435    0.774060   -0.369875
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5*E*

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Zero-point correction=                           0.253978 (Hartree/Particle)
 Thermal correction to Energy=                  0.266578
 Thermal correction to Enthalpy=                0.267522
 Thermal correction to Gibbs Free Energy=       0.212907
 Sum of electronic and zero-point Energies=          -578.982754
 Sum of electronic and thermal Energies=             -578.970154
 Sum of electronic and thermal Enthalpies=           -578.969209
 Sum of electronic and thermal Free Energies=        -579.023824

 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -1.682466   -1.461567   -0.014866
    2          6             0       -2.652210   -2.277015   -0.432119
    3          6             0       -1.865381   -0.047632    0.515186
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4	6	0	-0.197737	-1.766210	-0.043026
5	6	0	-2.681109	0.935946	-0.355845
6	6	0	-2.073512	2.305968	-0.011695
7	6	0	-0.554567	2.030948	0.060620
8	6	0	-0.431001	0.575204	0.582402
9	6	0	0.453537	-0.385290	-0.268376
10	6	0	1.906146	-0.335418	0.151956
11	8	0	2.341917	-0.768905	1.199016
12	8	0	2.676065	0.284422	-0.771908
13	6	0	4.065794	0.408934	-0.429631
14	1	0	-3.700523	-1.991276	-0.388451
15	1	0	-2.436097	-3.266385	-0.828384
16	1	0	-2.306527	-0.072677	1.520672
17	1	0	0.078590	-2.507315	-0.800846
18	1	0	0.137362	-2.148073	0.931781
19	1	0	-3.758543	0.879098	-0.166132
20	1	0	-2.524595	0.707590	-1.418097
21	1	0	-2.442081	2.639497	0.967849
22	1	0	-2.330733	3.086283	-0.736842
23	1	0	-0.112776	2.111127	-0.940708
24	1	0	-0.029316	2.752226	0.695612
25	1	0	-0.055968	0.552873	1.611269
26	1	0	0.380941	-0.105648	-1.324662
27	1	0	4.517756	-0.577374	-0.293831
28	1	0	4.185031	0.981758	0.494057
29	1	0	4.528652	0.930952	-1.267792

5 E_t

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Zero-point correction=                           0.253737 (Hartree/Particle)
 Thermal correction to Energy=                    0.266464
 Thermal correction to Enthalpy=                  0.267408
 Thermal correction to Gibbs Free Energy=         0.213191
 Sum of electronic and zero-point Energies=           -578.970922
 Sum of electronic and thermal Energies=              -578.958194
 Sum of electronic and thermal Enthalpies=            -578.957250
 Sum of electronic and thermal Free Energies=         -579.011467
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.652106	-1.484452	-0.182805
2	6	0	2.597730	-2.367054	0.138198
3	6	0	1.806498	0.000261	-0.388145
4	6	0	0.154681	-1.785366	-0.353249
5	6	0	2.833428	0.927838	0.263897
6	6	0	2.112214	2.323220	0.232149
7	6	0	0.606335	2.055295	-0.120878
8	6	0	0.470726	0.552486	0.123975
9	6	0	-0.553145	-0.400447	-0.527959
10	6	0	-1.911350	-0.345148	0.137878
11	8	0	-2.176920	-0.814370	1.225542
12	8	0	-2.806763	0.334852	-0.614514
13	6	0	-4.112024	0.480920	-0.032975
14	1	0	3.636469	-2.069212	0.256978
15	1	0	2.373377	-3.419892	0.294554
16	1	0	1.823005	0.187689	-1.477991
17	1	0	-0.241431	-2.282344	0.538851
18	1	0	-0.041705	-2.444641	-1.206973

19	1	0	3.798463	0.948222	-0.252568
20	1	0	3.020469	0.611479	1.297077
21	1	0	2.569370	2.989713	-0.506701
22	1	0	2.203368	2.823618	1.201791
23	1	0	-0.076561	2.666351	0.478067
24	1	0	0.411849	2.285668	-1.176311
25	1	0	0.430922	0.370537	1.209428
26	1	0	-0.668051	-0.145207	-1.586798
27	1	0	-4.054065	1.028708	0.911646
28	1	0	-4.560889	-0.498290	0.154439
29	1	0	-4.698322	1.038423	-0.764224

TS(2,4)*Z*

Zero-point correction= 0.305049 (Hartree/Particle)
Thermal correction to Energy= 0.325941
Thermal correction to Enthalpy= 0.326885
Thermal correction to Gibbs Free Energy= 0.255495
Sum of electronic and zero-point Energies= -1391.922993
Sum of electronic and thermal Energies= -1391.902102
Sum of electronic and thermal Enthalpies= -1391.901158
Sum of electronic and thermal Free Energies= -1391.972547

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.070073	-0.891194	0.238549
2	15	0	-1.973512	0.649387	1.802411
3	6	0	1.137244	-1.964016	0.234398
4	6	0	0.526491	-1.610479	1.497523
5	6	0	2.358174	-1.432347	-0.284825
6	6	0	0.107186	-2.505392	-0.616633
7	6	0	3.521905	-1.115037	0.647704
8	6	0	4.255313	0.116505	0.092766
9	6	0	3.151014	1.100078	-0.298876
10	6	0	2.135270	0.351372	-1.153595
11	6	0	0.804171	0.803574	-1.393018
12	15	0	-2.615157	-0.469722	-1.545992
13	6	0	0.025176	1.809331	-0.771110
14	8	0	-1.173296	2.062846	-1.027483
15	8	0	0.681486	2.593737	0.172120
16	6	0	0.040892	3.824186	0.493306
17	1	0	-1.129810	1.705580	2.198810
18	1	0	-3.146407	1.400239	1.562626
19	1	0	-2.318797	0.181444	3.094059
20	1	0	1.041826	-0.926435	2.168121
21	1	0	-0.046774	-2.385108	2.011429
22	1	0	2.671394	-1.977012	-1.176583
23	1	0	0.291351	-2.574128	-1.687486
24	1	0	-0.524027	-3.302372	-0.218088
25	1	0	4.199247	-1.973755	0.754822
26	1	0	3.150888	-0.883540	1.654140
27	1	0	4.840248	-0.165451	-0.795001
28	1	0	4.959187	0.541036	0.818976
29	1	0	2.670783	1.504846	0.595255
30	1	0	3.544151	1.957853	-0.861074
31	1	0	2.600399	-0.010883	-2.073773
32	1	0	0.290616	0.346832	-2.233735
33	1	0	-2.086667	-0.102779	-2.797108

34	1	0	-3.452368	-1.526339	-1.994397
35	1	0	-3.614967	0.518964	-1.436039
36	1	0	-0.929829	3.676572	0.978426
37	1	0	-0.119197	4.434075	-0.402574
38	1	0	0.719618	4.341009	1.176714

TS(2,4) Z_t

Zero-point correction= 0.303760 (Hartree/Particle)
Thermal correction to Energy= 0.325399
Thermal correction to Enthalpy= 0.326343
Thermal correction to Gibbs Free Energy= 0.251054
Sum of electronic and zero-point Energies= -1391.918649
Sum of electronic and thermal Energies= -1391.897011
Sum of electronic and thermal Enthalpies= -1391.896067
Sum of electronic and thermal Free Energies= -1391.971356

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.665318	-0.078593	-0.299149
2	15	0	-3.153750	-0.662138	1.447466
3	6	0	0.123246	-1.452773	-1.332465
4	6	0	-1.073182	-2.102709	-0.815677
5	6	0	1.443521	-1.637155	-0.875925
6	6	0	-0.309931	-0.221328	-1.965701
7	6	0	2.007440	-2.987046	-0.471205
8	6	0	3.115983	-2.771252	0.604513
9	6	0	3.063433	-1.302044	1.065541
10	6	0	1.629914	-0.796854	0.952258
11	6	0	1.220629	0.546825	1.091187
12	15	0	-1.748884	2.315591	-0.342548
13	6	0	1.859531	1.734775	0.626952
14	8	0	1.415181	2.888734	0.737126
15	8	0	3.064746	1.526799	-0.017570
16	6	0	3.718122	2.708424	-0.474847
17	1	0	-4.068993	-1.717656	1.224307
18	1	0	-2.600831	-1.159909	2.650613
19	1	0	-4.072491	0.239809	2.040182
20	1	0	-0.968667	-2.868045	-0.047579
21	1	0	-1.868451	-2.317186	-1.533214
22	1	0	2.163221	-1.001432	-1.392888
23	1	0	0.431026	0.557124	-2.138824
24	1	0	-1.073161	-0.295242	-2.743677
25	1	0	2.411943	-3.520988	-1.341648
26	1	0	1.209903	-3.624285	-0.070265
27	1	0	4.106589	-3.015806	0.205190
28	1	0	2.952588	-3.446786	1.453106
29	1	0	3.393988	-1.202978	2.108621
30	1	0	3.723046	-0.670464	0.467249
31	1	0	0.935563	-1.477652	1.456166
32	1	0	0.254951	0.734120	1.550737
33	1	0	-0.551882	2.894083	0.157912
34	1	0	-1.841494	2.966706	-1.594070
35	1	0	-2.714219	3.095452	0.342245
36	1	0	3.103696	3.249201	-1.202486
37	1	0	4.645491	2.371313	-0.943930
38	1	0	3.940684	3.386665	0.355130

TS(2,4)*E*

Zero-point correction= 0.304264 (Hartree/Particle)
Thermal correction to Energy= 0.325552
Thermal correction to Enthalpy= 0.326496
Thermal correction to Gibbs Free Energy= 0.252666
Sum of electronic and zero-point Energies= -1391.929302
Sum of electronic and thermal Energies= -1391.908013
Sum of electronic and thermal Enthalpies= -1391.907069
Sum of electronic and thermal Free Energies= -1391.980899

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.028156	-0.816038	-0.325422
2	15	0	-1.806803	-2.267735	1.381214
3	6	0	1.167701	-0.841563	-1.479766
4	6	0	0.591468	-2.082486	-1.027547
5	6	0	2.396475	-0.280372	-1.033508
6	6	0	0.087036	-0.024463	-1.999509
7	6	0	3.563504	-1.179101	-0.639456
8	6	0	4.224503	-0.607982	0.627778
9	6	0	3.074640	-0.139764	1.520244
10	6	0	2.128636	0.716380	0.690690
11	6	0	0.803183	0.931836	1.144856
12	15	0	-2.837390	0.788209	-0.344496
13	6	0	0.018228	2.065920	0.807247
14	8	0	-1.136717	2.319569	1.193640
15	8	0	0.656703	2.944655	-0.060131
16	6	0	-0.051172	4.146393	-0.340401
17	1	0	-1.263053	-2.093854	2.675344
18	1	0	-3.164629	-2.356834	1.779107
19	1	0	-1.572308	-3.659623	1.276283
20	1	0	1.144352	-2.724309	-0.344837
21	1	0	-0.039153	-2.630450	-1.731389
22	1	0	2.688838	0.582284	-1.631447
23	1	0	0.243538	1.049863	-2.072893
24	1	0	-0.535229	-0.451042	-2.789339
25	1	0	4.290225	-1.274401	-1.457801
26	1	0	3.206333	-2.194404	-0.426528
27	1	0	4.854727	0.253932	0.366384
28	1	0	4.874024	-1.341090	1.121356
29	1	0	2.531934	-1.005861	1.926872
30	1	0	3.438992	0.438061	2.380539
31	1	0	2.605363	1.618025	0.309420
32	1	0	0.362865	0.263994	1.879725
33	1	0	-2.720572	2.048177	-0.958187
34	1	0	-3.941855	0.318602	-1.109279
35	1	0	-3.566035	1.157588	0.803179
36	1	0	-0.320807	4.676788	0.578286
37	1	0	-0.971128	3.955327	-0.905841
38	1	0	0.626554	4.757296	-0.942125

TS(2,4)*Z´*

Zero-point correction= 0.276455 (Hartree/Particle)
Thermal correction to Energy= 0.294528

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 Thermal correction to Enthalpy=                  0.295472
 Thermal correction to Gibbs Free Energy=         0.229627
 Sum of electronic and zero-point Energies=          -1048.791230
 Sum of electronic and thermal Energies=             -1048.773157
 Sum of electronic and thermal Enthalpies=           -1048.772213
 Sum of electronic and thermal Free Energies=        -1048.838058

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 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         46             0       -0.276669   -1.238650   -0.323565
    2         15             0       -1.679949   -1.426876    1.583701
    3          6             0        2.074301   -1.032591   -0.571826
    4          6             0        1.613234   -1.879198    0.494584
    5          6             0        2.690114    0.227155   -0.436749
    6          6             0        1.313337   -1.392790   -1.764962
    7          6             0        3.268137    0.780811    0.841567
    8          6             0        2.849459    2.258088    0.979505
    9          6             0        1.345270    2.350847    0.701161
   10          6             0        1.026937    1.735629   -0.642894
   11          6             0       -0.250616    1.289719   -1.050760
   12          6             0       -1.462988    1.454888   -0.258616
   13          8             0       -1.576271    1.613903    0.956547
   14          8             0       -2.569810    1.463322   -1.075612
   15          6             0       -3.814222    1.710291   -0.423687
   16          1             0       -1.264048   -0.854150    2.805144
   17          1             0       -3.003656   -0.935446    1.583087
   18          1             0       -1.965255   -2.723669    2.079557
   19          1             0        1.800201   -1.624351    1.535234
   20          1             0        1.544025   -2.948655    0.297138
   21          1             0        3.147757    0.598248   -1.351413
   22          1             0        1.322744   -0.705430   -2.608218
   23          1             0        1.279180   -2.446362   -2.047740
   24          1             0        4.364359    0.692649    0.868432
   25          1             0        2.890196    0.225398    1.709072
   26          1             0        3.397392    2.863838    0.242721
   27          1             0        3.102985    2.657875    1.969059
   28          1             0        0.768830    1.857199    1.487531
   29          1             0        1.020812    3.402808    0.700033
   30          1             0        1.622746    2.139306   -1.459326
   31          1             0       -0.433448    1.231441   -2.118903
   32          1             0       -3.777148    2.632496    0.163586
   33          1             0       -4.087418    0.885782    0.244418
   34          1             0       -4.553397    1.797161   -1.222355
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TS(2,4)Z_t´

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Zero-point correction=                           0.275921 (Hartree/Particle)
 Thermal correction to Energy=                   0.294480
 Thermal correction to Enthalpy=                 0.295424
 Thermal correction to Gibbs Free Energy=        0.227074
 Sum of electronic and zero-point Energies=          -1048.781169
 Sum of electronic and thermal Energies=             -1048.762610
 Sum of electronic and thermal Enthalpies=           -1048.761665
 Sum of electronic and thermal Free Energies=        -1048.830016

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

1	46	0	-1.466913	-0.408690	0.331232
2	15	0	-3.164453	-0.628901	-1.307476
3	6	0	-0.256624	1.421707	1.375864
4	6	0	-1.622599	1.654863	0.976716
5	6	0	0.899471	1.960009	0.809753
6	6	0	-0.238428	0.092221	1.995631
7	6	0	1.059469	3.256745	0.062607
8	6	0	2.238492	3.086063	-0.941960
9	6	0	2.473087	1.580326	-1.214983
10	6	0	1.181169	0.802820	-1.039114
11	6	0	1.046495	-0.581197	-0.886519
12	6	0	2.020890	-1.407049	-0.198014
13	8	0	2.943049	-1.017537	0.512146
14	8	0	1.786547	-2.743679	-0.400456
15	6	0	2.680636	-3.623356	0.282112
16	1	0	-4.267395	-1.468326	-1.017356
17	1	0	-3.916576	0.501525	-1.710647
18	1	0	-2.913104	-1.130582	-2.609296
19	1	0	-1.853958	2.371064	0.189051
20	1	0	-2.400874	1.549820	1.732004
21	1	0	1.815804	1.588623	1.265647
22	1	0	0.723586	-0.410657	2.073937
23	1	0	-0.913586	-0.079621	2.836617
24	1	0	1.259424	4.100734	0.738011
25	1	0	0.135223	3.510342	-0.473791
26	1	0	3.153389	3.534907	-0.539099
27	1	0	2.018621	3.622078	-1.873057
28	1	0	2.828040	1.434748	-2.246168
29	1	0	3.238743	1.162907	-0.558181
30	1	0	0.347409	1.254241	-1.583481
31	1	0	0.260854	-1.107235	-1.424472
32	1	0	3.717782	-3.438691	-0.014086
33	1	0	2.378720	-4.632944	-0.003522
34	1	0	2.603581	-3.498866	1.367295

TS(2,4)*E´*

Zero-point correction= 0.276134 (Hartree/Particle)
Thermal correction to Energy= 0.294321
Thermal correction to Enthalpy= 0.295266
Thermal correction to Gibbs Free Energy= 0.228622
Sum of electronic and zero-point Energies= -1048.796454
Sum of electronic and thermal Energies= -1048.778266
Sum of electronic and thermal Enthalpies= -1048.777322
Sum of electronic and thermal Free Energies= -1048.843966

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.312261	1.158207	-0.338877
2	15	0	0.546896	2.876290	1.264313
3	6	0	-1.484045	0.082014	-1.499589
4	6	0	-1.666932	1.470188	-1.178432
5	6	0	-2.146567	-1.015521	-0.923208
6	6	0	-0.138720	-0.046770	-2.058543
7	6	0	-3.379288	-0.931613	-0.060415
8	6	0	-3.191639	-1.847411	1.165614
9	6	0	-1.798122	-1.587970	1.750446

10	6	0	-0.726808	-1.738988	0.696720
11	6	0	0.524562	-1.109512	0.802019
12	6	0	1.676988	-1.708529	0.135652
13	8	0	1.648167	-2.588198	-0.715895
14	8	0	2.859735	-1.175818	0.584231
15	6	0	4.033870	-1.715566	-0.025732
16	1	0	-0.517825	3.760194	1.571370
17	1	0	0.929852	2.613826	2.603768
18	1	0	1.520111	3.872358	1.006941
19	1	0	-2.432362	1.792402	-0.475740
20	1	0	-1.420850	2.202886	-1.946207
21	1	0	-2.001400	-1.956658	-1.447976
22	1	0	0.318782	-1.033159	-2.092745
23	1	0	0.128551	0.614408	-2.885480
24	1	0	-4.288164	-1.219787	-0.609075
25	1	0	-3.540249	0.097239	0.286474
26	1	0	-3.256786	-2.898235	0.849518
27	1	0	-3.979380	-1.691772	1.913322
28	1	0	-1.752856	-0.579727	2.186028
29	1	0	-1.599315	-2.293216	2.571940
30	1	0	-0.707339	-2.694539	0.178151
31	1	0	0.733744	-0.468807	1.656047
32	1	0	4.042656	-1.519060	-1.102745
33	1	0	4.097323	-2.796711	0.130137
34	1	0	4.875064	-1.213338	0.456051

TS(2,4)E_t'

Zero-point correction= 0.276032 (Hartree/Particle)
Thermal correction to Energy= 0.294360
Thermal correction to Enthalpy= 0.295305
Thermal correction to Gibbs Free Energy= 0.228528
Sum of electronic and zero-point Energies= -1048.774652
Sum of electronic and thermal Energies= -1048.756324
Sum of electronic and thermal Enthalpies= -1048.755379
Sum of electronic and thermal Free Energies= -1048.822156

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.869413	-1.139054	-0.393402
2	15	0	-2.557838	-0.753047	1.234901
3	6	0	1.494294	-1.653495	-0.293886
4	6	0	0.625180	-2.169900	0.737702
5	6	0	2.489545	-0.680465	-0.141959
6	6	0	0.777096	-1.821944	-1.555485
7	6	0	3.335997	-0.421173	1.079588
8	6	0	3.845282	1.046879	0.991178
9	6	0	2.921504	1.837954	0.035327
10	6	0	1.528634	1.228239	0.010831
11	6	0	0.586633	1.492608	-0.990311
12	6	0	-0.765451	1.971620	-0.780196
13	8	0	-1.511659	2.399668	-1.651555
14	8	0	-1.150205	2.038343	0.561437
15	6	0	-2.304551	2.848226	0.789439
16	1	0	-3.370853	-1.828128	1.670331
17	1	0	-2.187879	-0.283561	2.515607
18	1	0	-3.601566	0.168794	0.994009
19	1	0	0.745345	-1.839765	1.768858

20	1	0	0.258322	-3.191462	0.633847
21	1	0	3.001126	-0.455158	-1.077912
22	1	0	1.091584	-1.218387	-2.404678
23	1	0	0.437934	-2.826673	-1.816187
24	1	0	4.183916	-1.116564	1.149924
25	1	0	2.745951	-0.565840	1.994017
26	1	0	4.878493	1.075970	0.627359
27	1	0	3.856840	1.505129	1.986757
28	1	0	2.838891	2.885300	0.358029
29	1	0	3.330254	1.865431	-0.982198
30	1	0	1.103854	1.116388	1.010234
31	1	0	0.924612	1.653276	-2.011832
32	1	0	-2.122034	3.883266	0.482038
33	1	0	-2.489761	2.808322	1.865716
34	1	0	-3.174521	2.480475	0.236638

TS(2,6)*Z*

Zero-point correction= 0.304963 (Hartree/Particle)
Thermal correction to Energy= 0.325829
Thermal correction to Enthalpy= 0.326773
Thermal correction to Gibbs Free Energy= 0.255710
Sum of electronic and zero-point Energies= -1391.925449
Sum of electronic and thermal Energies= -1391.904583
Sum of electronic and thermal Enthalpies= -1391.903639
Sum of electronic and thermal Free Energies= -1391.974702

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.700703	-1.092963	0.111095
2	15	0	-1.466328	-0.287863	2.221457
3	6	0	1.633152	-1.559435	-0.432170
4	6	0	1.154656	-1.815341	0.912354
5	6	0	2.652250	-0.628378	-0.790092
6	6	0	0.616363	-2.013901	-1.351314
7	6	0	3.829840	-0.411510	0.162202
8	6	0	4.077125	1.098577	0.356462
9	6	0	2.699625	1.759624	0.332135
10	6	0	1.982529	1.259126	-0.912651
11	6	0	0.607344	1.511821	-1.170421
12	15	0	-2.540596	-0.673653	-1.360748
13	6	0	-0.363969	1.924862	-0.230270
14	8	0	-0.294229	2.062192	1.004111
15	8	0	-1.579265	2.234349	-0.874951
16	6	0	-2.528251	2.928799	-0.076427
17	1	0	-0.514345	0.307446	3.067021
18	1	0	-2.515472	0.642051	2.377667
19	1	0	-1.960419	-1.263917	3.127271
20	1	0	1.618359	-1.306413	1.753821
21	1	0	0.824039	-2.831649	1.138840
22	1	0	2.939426	-0.733667	-1.836032
23	1	0	0.646168	-1.660364	-2.380660
24	1	0	0.240117	-3.031900	-1.234253
25	1	0	4.732546	-0.915819	-0.207826
26	1	0	3.607366	-0.862164	1.136666
27	1	0	4.683679	1.491134	-0.472416
28	1	0	4.631748	1.303330	1.280099
29	1	0	2.117878	1.518865	1.226656

30	1	0	2.774480	2.854926	0.295038
31	1	0	2.589402	1.433533	-1.804390
32	1	0	0.280719	1.509755	-2.206245
33	1	0	-2.272785	-0.019306	-2.578983
34	1	0	-3.197243	-1.812744	-1.891284
35	1	0	-3.707392	0.039925	-0.999860
36	1	0	-2.067024	3.768280	0.452294
37	1	0	-2.997581	2.275256	0.670118
38	1	0	-3.293513	3.294673	-0.766649

TS(2,6) E_t

Zero-point correction= 0.304852 (Hartree/Particle)
Thermal correction to Energy= 0.325928
Thermal correction to Enthalpy= 0.326872
Thermal correction to Gibbs Free Energy= 0.254233
Sum of electronic and zero-point Energies= -1391.928681
Sum of electronic and thermal Energies= -1391.907605
Sum of electronic and thermal Enthalpies= -1391.906661
Sum of electronic and thermal Free Energies= -1391.979300

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.504774	-1.383984	-0.147323
2	15	0	-0.980369	-1.599824	2.164980
3	6	0	1.625116	-0.984206	-1.165407
4	6	0	1.576821	-2.031365	-0.161525
5	6	0	2.394095	0.202337	-1.067671
6	6	0	0.475741	-1.152390	-2.038215
7	6	0	3.816918	0.131266	-0.510259
8	6	0	3.903986	0.828079	0.862874
9	6	0	2.921264	1.992545	0.815598
10	6	0	1.559179	1.493334	0.361211
11	6	0	0.601735	2.403984	-0.112382
12	15	0	-2.619028	-0.603556	-0.888019
13	6	0	-0.786688	2.263794	0.130858
14	8	0	-1.387597	1.355345	0.748008
15	8	0	-1.506541	3.331293	-0.376037
16	6	0	-2.875030	3.397988	-0.001105
17	1	0	-0.910350	-2.831157	2.862862
18	1	0	-0.157148	-0.849093	3.031544
19	1	0	-2.227656	-1.170779	2.673296
20	1	0	2.187681	-1.935716	0.734352
21	1	0	1.442750	-3.058373	-0.503244
22	1	0	2.278106	0.862723	-1.924293
23	1	0	0.196372	-0.326419	-2.690643
24	1	0	0.317965	-2.140993	-2.471257
25	1	0	4.488736	0.643954	-1.210958
26	1	0	4.173092	-0.904910	-0.443985
27	1	0	4.926373	1.149011	1.096695
28	1	0	3.599563	0.132486	1.658451
29	1	0	2.811153	2.465274	1.802007
30	1	0	3.278398	2.774262	0.130794
31	1	0	1.152489	0.705258	0.996389
32	1	0	0.919891	3.310063	-0.620595
33	1	0	-2.654551	0.548735	-1.697128
34	1	0	-3.383438	-1.447201	-1.737342
35	1	0	-3.653407	-0.273485	0.013811

36	1	0	-3.470640	2.609285	-0.477763
37	1	0	-3.230548	4.372987	-0.343540
38	1	0	-2.999982	3.312718	1.083379

TS(2,6)*Z´*

Zero-point correction= 0.276102 (Hartree/Particle)
Thermal correction to Energy= 0.294080
Thermal correction to Enthalpy= 0.295025
Thermal correction to Gibbs Free Energy= 0.229824
Sum of electronic and zero-point Energies= -1048.783691
Sum of electronic and thermal Energies= -1048.765712
Sum of electronic and thermal Enthalpies= -1048.764768
Sum of electronic and thermal Free Energies= -1048.829969

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.738842	-0.899293	-0.419721
2	6	0	-1.491748	-1.562132	0.129898
3	6	0	-1.164585	-1.441093	-1.262412
4	6	0	-2.441163	-0.748318	0.797188
5	6	0	-0.364890	-2.273982	0.741939
6	6	0	-3.736297	-0.403877	0.062152
7	6	0	-3.919195	1.122551	-0.090836
8	6	0	-2.525783	1.734940	-0.211796
9	6	0	-1.690804	1.241504	0.955010
10	6	0	-0.309309	1.506378	1.095866
11	15	0	2.872013	-0.981994	0.694252
12	6	0	0.632545	1.723487	0.056457
13	8	0	0.575687	1.379097	-1.156329
14	8	0	1.765934	2.368222	0.505431
15	6	0	2.718654	2.719745	-0.497871
16	1	0	-1.645757	-0.694158	-1.886643
17	1	0	-0.797062	-2.321862	-1.793135
18	1	0	-2.543949	-0.963089	1.859980
19	1	0	-0.232278	-2.201742	1.821126
20	1	0	-0.124656	-3.256194	0.331799
21	1	0	-4.598619	-0.844506	0.579650
22	1	0	-3.718076	-0.860023	-0.935042
23	1	0	-4.412397	1.536128	0.800202
24	1	0	-4.559919	1.365899	-0.946747
25	1	0	-2.045195	1.484479	-1.163090
26	1	0	-2.575622	2.832446	-0.165829
27	1	0	-2.220141	1.362402	1.901602
28	1	0	0.072904	1.673717	2.098695
29	1	0	2.904841	-0.722819	2.083833
30	1	0	3.530757	-2.234034	0.738692
31	1	0	4.010703	-0.210280	0.350124
32	1	0	2.287568	3.416767	-1.223270
33	1	0	3.080593	1.840798	-1.040884
34	1	0	3.541885	3.199662	0.035937

TS(2,6)E_t´

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Zero-point correction=                           0.276269 (Hartree/Particle)
 Thermal correction to Energy=                    0.294218
 Thermal correction to Enthalpy=                  0.295162
 Thermal correction to Gibbs Free Energy=         0.229519
 Sum of electronic and zero-point Energies=          -1048.802049
 Sum of electronic and thermal Energies=             -1048.784100
 Sum of electronic and thermal Enthalpies=           -1048.783156
 Sum of electronic and thermal Free Energies=        -1048.848799

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         46             0       -0.467530   -1.122802   -0.322640
    2         15             0       -0.966501   -2.600152    1.471577
    3          6             0        1.473298   -0.375098   -1.435684
    4          6             0        1.457376   -1.762681   -0.952132
    5          6             0        2.211298    0.716859   -0.935048
    6          6             0        0.224494   -0.172081   -2.126526
    7          6             0        3.521796    0.611576   -0.181332
    8          6             0        3.355908    1.125399    1.276168
    9          6             0        2.184789    2.112347    1.315911
   10          6             0        0.969323    1.470525    0.679676
   11          6             0       -0.157380    2.204646    0.291897
   12          6             0       -1.474742    1.683767    0.161728
   13          8             0       -1.895578    0.492672    0.220838
   14          8             0       -2.397812    2.670263   -0.024127
   15          6             0       -3.753136    2.254613   -0.190487
   16          1             0       -1.493201   -2.115531    2.694759
   17          1             0       -1.946754   -3.597345    1.247563
   18          1             0        0.015236   -3.453857    2.030218
   19          1             0        2.143343   -2.054075   -0.157324
   20          1             0        1.313136   -2.535005   -1.708473
   21          1             0        2.089659    1.627756   -1.515809
   22          1             0       -0.114474    0.843673   -2.317857
   23          1             0       -0.108877   -0.919461   -2.846820
   24          1             0        4.279405    1.220539   -0.692431
   25          1             0        3.907133   -0.415901   -0.178912
   26          1             0        4.280729    1.575717    1.655687
   27          1             0        3.122900    0.282590    1.942126
   28          1             0        1.948149    2.385134    2.355084
   29          1             0        2.434625    3.046656    0.795187
   30          1             0        0.767465    0.467556    1.060383
   31          1             0       -0.061854    3.271299    0.108491
   32          1             0       -3.858642    1.574148   -1.041320
   33          1             0       -4.318038    3.171787   -0.368831
   34          1             0       -4.127079    1.752772    0.707349
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6(E,Z)

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Zero-point correction=                           0.307434 (Hartree/Particle)
 Thermal correction to Energy=                    0.328347
 Thermal correction to Enthalpy=                  0.329291
 Thermal correction to Gibbs Free Energy=         0.257091
 Sum of electronic and zero-point Energies=          -1391.932125
 Sum of electronic and thermal Energies=             -1391.911213
 Sum of electronic and thermal Enthalpies=           -1391.910268
 Sum of electronic and thermal Free Energies=        -1391.982468

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.517962	-1.120088	0.207117
2	15	0	-1.369078	-0.028410	2.139103
3	6	0	1.683732	-1.357206	-0.355722
4	6	0	1.453694	-1.466646	1.049591
5	6	0	2.467777	-0.224696	-0.982485
6	6	0	0.903448	-2.234122	-1.136344
7	6	0	3.868107	-0.057649	-0.310890
8	6	0	3.840366	1.281348	0.487689
9	6	0	2.383109	1.776141	0.446168
10	6	0	1.842323	1.245312	-0.893274
11	6	0	0.391836	1.429659	-1.215333
12	15	0	-2.450003	-1.085695	-1.164006
13	6	0	-0.614019	1.792981	-0.350453
14	8	0	-0.612113	1.998151	0.902484
15	8	0	-1.884046	1.876653	-1.016834
16	6	0	-2.772046	2.846045	-0.484136
17	1	0	-0.544214	0.678935	3.025380
18	1	0	-2.544434	0.740685	2.135420
19	1	0	-1.825922	-1.012023	3.073955
20	1	0	1.898034	-0.747009	1.728054
21	1	0	1.260496	-2.448863	1.481144
22	1	0	2.576684	-0.478737	-2.041868
23	1	0	0.869481	-2.112500	-2.215396
24	1	0	0.636761	-3.220533	-0.759795
25	1	0	4.648909	-0.038484	-1.078480
26	1	0	4.098472	-0.909239	0.338615
27	1	0	4.497654	2.013586	0.003528
28	1	0	4.214963	1.155233	1.510069
29	1	0	1.789359	1.390717	1.278437
30	1	0	2.302711	2.866421	0.500774
31	1	0	2.417394	1.771026	-1.675558
32	1	0	0.125121	1.396164	-2.268700
33	1	0	-2.344908	-0.459894	-2.418015
34	1	0	-2.981497	-2.330101	-1.588036
35	1	0	-3.659409	-0.508725	-0.724988
36	1	0	-2.468052	3.863503	-0.772059
37	1	0	-2.815157	2.797691	0.608422
38	1	0	-3.760669	2.642333	-0.908795

6 (*E*,Z)$_t$

Zero-point correction= 0.307791 (Hartree/Particle)
Thermal correction to Energy= 0.328541
Thermal correction to Enthalpy= 0.329485
Thermal correction to Gibbs Free Energy= 0.257987
Sum of electronic and zero-point Energies= -1391.940465
Sum of electronic and thermal Energies= -1391.919715
Sum of electronic and thermal Enthalpies= -1391.918771
Sum of electronic and thermal Free Energies= -1391.990269

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.449684	-1.362678	-0.105545
2	15	0	-1.179171	-1.227276	2.134505
3	6	0	1.643709	-1.086430	-0.895441

4	6	0	1.630096	-1.959754	0.228555
5	6	0	2.270233	0.283135	-0.840691
6	6	0	0.763425	-1.473690	-1.940062
7	6	0	3.789718	0.232978	-0.464469
8	6	0	3.945930	1.089745	0.810503
9	6	0	2.806481	2.106896	0.708020
10	6	0	1.590512	1.293915	0.202194
11	6	0	0.475366	2.122162	-0.335980
12	15	0	-2.483138	-0.569741	-1.029516
13	6	0	-0.844189	1.998853	0.013223
14	8	0	-1.427506	1.168730	0.800861
15	8	0	-1.686141	2.901743	-0.674477
16	6	0	-2.840355	3.313828	0.036009
17	1	0	-1.254648	-2.364791	2.982999
18	1	0	-0.414659	-0.399487	2.975007
19	1	0	-2.458940	-0.699341	2.377836
20	1	0	2.136470	-1.665295	1.144047
21	1	0	1.527369	-3.033361	0.079216
22	1	0	2.157824	0.736125	-1.829951
23	1	0	0.573659	-0.786229	-2.759268
24	1	0	0.599502	-2.528426	-2.156547
25	1	0	4.374270	0.668157	-1.283197
26	1	0	4.158562	-0.789653	-0.327278
27	1	0	4.940244	1.544370	0.887330
28	1	0	3.807566	0.466776	1.705576
29	1	0	2.583045	2.615781	1.651874
30	1	0	3.056636	2.884576	-0.027680
31	1	0	1.221974	0.694522	1.044663
32	1	0	0.735164	2.932207	-1.013060
33	1	0	-2.424586	0.674068	-1.681953
34	1	0	-3.111797	-1.327909	-2.055778
35	1	0	-3.616435	-0.393341	-0.211967
36	1	0	-3.463468	2.467712	0.347125
37	1	0	-3.406722	3.956354	-0.645203
38	1	0	-2.577301	3.892031	0.934199

6(E,*Z*)´

Zero-point correction= 0.279364 (Hartree/Particle)
Thermal correction to Energy= 0.297249
Thermal correction to Enthalpy= 0.298193
Thermal correction to Gibbs Free Energy= 0.233092
Sum of electronic and zero-point Energies= -1048.808468
Sum of electronic and thermal Energies= -1048.790584
Sum of electronic and thermal Enthalpies= -1048.789639
Sum of electronic and thermal Free Energies= -1048.854741

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.656707	-0.919251	-0.346980
2	6	0	-1.426895	-1.340733	0.070426
3	6	0	-1.299481	-1.212469	-1.324136
4	6	0	-2.133690	-0.314305	0.948721
5	6	0	-0.618089	-2.396982	0.619301
6	6	0	-3.644196	-0.244380	0.594016
7	6	0	-3.773439	0.840458	-0.511880
8	6	0	-2.504834	1.729543	-0.398325
9	6	0	-1.735817	1.213435	0.846934

10	6	0	-0.311394	1.693277	1.018908
11	15	0	2.843884	-1.110004	0.561443
12	6	0	0.714731	1.669832	0.110998
13	8	0	0.744959	1.130459	-1.074393
14	8	0	1.909508	2.237237	0.568175
15	6	0	2.742430	2.792973	-0.443240
16	1	0	-1.671308	-0.348064	-1.856523
17	1	0	-1.047382	-2.078637	-1.933019
18	1	0	-1.994475	-0.642236	1.984865
19	1	0	-0.544677	-2.502930	1.698384
20	1	0	-0.482430	-3.316081	0.052428
21	1	0	-4.190406	0.069602	1.491547
22	1	0	-4.059676	-1.211706	0.291090
23	1	0	-4.695616	1.416456	-0.379850
24	1	0	-3.842221	0.376174	-1.502609
25	1	0	-1.869134	1.657967	-1.285387
26	1	0	-2.748379	2.790552	-0.278169
27	1	0	-2.272240	1.627459	1.712974
28	1	0	-0.090912	2.214634	1.945450
29	1	0	3.054155	-0.678341	1.888784
30	1	0	3.459672	-2.378446	0.678917
31	1	0	3.932112	-0.431205	-0.033552
32	1	0	2.252441	3.641707	-0.940050
33	1	0	3.011015	2.054580	-1.204711
34	1	0	3.640978	3.148663	0.068259

6(*E*,Z)$_t$´

Zero-point correction= 0.278943 (Hartree/Particle)
Thermal correction to Energy= 0.296976
Thermal correction to Enthalpy= 0.297920
Thermal correction to Gibbs Free Energy= 0.231903
Sum of electronic and zero-point Energies= -1048.821224
Sum of electronic and thermal Energies= -1048.803191
Sum of electronic and thermal Enthalpies= -1048.802247
Sum of electronic and thermal Free Energies= -1048.868264

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.658859	-0.991096	0.284675
2	15	0	1.563582	-2.237561	-1.499514
3	6	0	-1.202994	-0.687251	1.389606
4	6	0	-1.036580	-2.085341	1.096957
5	6	0	-2.120031	0.273651	0.651552
6	6	0	-0.159270	-0.150505	2.163234
7	6	0	-3.325477	-0.330646	-0.081852
8	6	0	-3.836960	0.817376	-0.987124
9	6	0	-2.622399	1.765440	-1.195096
10	6	0	-1.404316	1.107621	-0.496736
11	6	0	-0.322307	2.086713	-0.144444
12	6	0	1.029470	1.860626	-0.150388
13	8	0	1.704903	0.749368	-0.308622
14	8	0	1.806291	2.990138	0.031091
15	6	0	3.198926	2.792586	0.222064
16	1	0	1.169702	-1.871603	-2.805781
17	1	0	2.960371	-2.131998	-1.684688
18	1	0	1.448763	-3.639410	-1.653019
19	1	0	-1.702400	-2.578319	0.395487

20	1	0	-0.628268	-2.732309	1.871403
21	1	0	-2.482332	0.999623	1.392797
22	1	0	-0.054977	0.925274	2.258915
23	1	0	0.386188	-0.772256	2.871014
24	1	0	-4.094852	-0.717060	0.596508
25	1	0	-2.994771	-1.171063	-0.705862
26	1	0	-4.661863	1.349101	-0.499314
27	1	0	-4.231964	0.430333	-1.932491
28	1	0	-2.409204	1.959729	-2.251234
29	1	0	-2.815575	2.740390	-0.731182
30	1	0	-0.999743	0.342490	-1.181269
31	1	0	-0.626884	3.112516	0.044332
32	1	0	3.410335	2.158061	1.091612
33	1	0	3.613690	3.790418	0.390186
34	1	0	3.674613	2.342263	-0.656165

7*z*

Zero-point correction= 0.305761 (Hartree/Particle)
Thermal correction to Energy= 0.327534
Thermal correction to Enthalpy= 0.328478
Thermal correction to Gibbs Free Energy= 0.253842
Sum of electronic and zero-point Energies= -1391.935043
Sum of electronic and thermal Energies= -1391.913270
Sum of electronic and thermal Enthalpies= -1391.912326
Sum of electronic and thermal Free Energies= -1391.986961

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.230591	-0.265539	-0.087134
2	15	0	-3.051738	-1.623945	-0.493030
3	6	0	1.327824	-1.150865	-1.417263
4	6	0	-0.051615	-1.592315	-1.316517
5	6	0	2.334309	-1.394502	-0.306460
6	6	0	1.742476	-0.439616	-2.498280
7	6	0	1.846240	-2.116054	0.969518
8	6	0	2.774967	-1.601693	2.080754
9	6	0	2.892895	-0.105925	1.759676
10	6	0	3.031660	-0.037539	0.212266
11	6	0	2.552404	1.229606	-0.433319
12	15	0	-2.251717	1.274822	1.700389
13	6	0	1.266347	1.696042	-0.326591
14	8	0	0.336457	1.169083	0.396105
15	8	0	0.985171	2.829286	-1.069313
16	6	0	-0.207842	3.525739	-0.760931
17	1	0	-2.922910	-2.767161	-1.320656
18	1	0	-3.736258	-2.256249	0.575825
19	1	0	-4.199841	-1.078190	-1.120165
20	1	0	-0.193665	-2.529317	-0.773432
21	1	0	-0.571131	-1.608731	-2.277624
22	1	0	3.139206	-2.003610	-0.739061
23	1	0	1.056546	-0.162736	-3.295458
24	1	0	2.784011	-0.175714	-2.644276
25	1	0	1.860280	-3.208429	0.868087
26	1	0	0.816226	-1.817743	1.203149
27	1	0	3.757257	-2.090932	2.010457
28	1	0	2.385246	-1.798378	3.086790
29	1	0	1.974522	0.408035	2.057901

30	1	0	3.733518	0.383550	2.264788
31	1	0	4.098378	-0.130649	-0.024680
32	1	0	3.252482	1.838169	-0.995645
33	1	0	-1.374706	1.345494	2.805122
34	1	0	-2.326624	2.665707	1.454634
35	1	0	-3.456226	1.191812	2.454451
36	1	0	-0.243001	3.830617	0.293637
37	1	0	-1.102933	2.933162	-0.985747
38	1	0	-0.202404	4.418718	-1.391783

7*E*

Zero-point correction= 0.305520 (Hartree/Particle)
Thermal correction to Energy= 0.327405
Thermal correction to Enthalpy= 0.328349
Thermal correction to Gibbs Free Energy= 0.253248
Sum of electronic and zero-point Energies= -1391.938732
Sum of electronic and thermal Energies= -1391.916847
Sum of electronic and thermal Enthalpies= -1391.915903
Sum of electronic and thermal Free Energies= -1391.991004

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.397263	-0.439945	-0.030624
2	15	0	2.941564	-2.120851	0.306329
3	6	0	-1.381624	-1.087837	0.975179
4	6	0	-0.076469	-1.718547	0.910800
5	6	0	-2.247967	-1.066003	-0.262790
6	6	0	-1.790649	-0.424092	2.087876
7	6	0	-3.636900	-1.733945	-0.120483
8	6	0	-4.496909	-1.048792	-1.191339
9	6	0	-4.096868	0.428212	-1.054243
10	6	0	-2.570677	0.426215	-0.777452
11	6	0	-2.127582	1.523178	0.138894
12	15	0	2.829557	1.156335	-1.452945
13	6	0	-0.800377	1.848309	0.262832
14	8	0	0.151356	1.310128	-0.419727
15	8	0	-0.499380	2.828250	1.189774
16	6	0	0.819732	3.342444	1.175046
17	1	0	4.088024	-1.858086	1.097657
18	1	0	2.559799	-3.329172	0.941076
19	1	0	3.630496	-2.705585	-0.786712
20	1	0	-0.030685	-2.577348	0.234958
21	1	0	0.353854	-1.954151	1.887520
22	1	0	-1.712913	-1.581374	-1.069415
23	1	0	-1.150358	-0.329570	2.961652
24	1	0	-2.790556	-0.016304	2.178812
25	1	0	-4.052528	-1.525392	0.874007
26	1	0	-3.587796	-2.824066	-0.228416
27	1	0	-5.571590	-1.219074	-1.057517
28	1	0	-4.227447	-1.427039	-2.187540
29	1	0	-4.358618	1.031252	-1.931003
30	1	0	-4.626225	0.866128	-0.196558
31	1	0	-2.029821	0.530737	-1.725648
32	1	0	-2.856013	2.102349	0.696891
33	1	0	2.100783	1.533473	-2.602219
34	1	0	3.071351	2.462708	-0.967516
35	1	0	4.088309	1.002915	-2.100484

36	1	0	1.072965	3.792053	0.205627
37	1	0	1.564625	2.572559	1.409639
38	1	0	0.845367	4.116315	1.946794

TS(7,5)*Z*

Zero-point correction= 0.304994 (Hartree/Particle)
Thermal correction to Energy= 0.326309
Thermal correction to Enthalpy= 0.327254
Thermal correction to Gibbs Free Energy= 0.253333
Sum of electronic and zero-point Energies= -1391.935320
Sum of electronic and thermal Energies= -1391.914004
Sum of electronic and thermal Enthalpies= -1391.913060
Sum of electronic and thermal Free Energies= -1391.986981

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.254926	-0.258817	-0.083226
2	15	0	-3.128128	-1.535420	-0.547684
3	6	0	1.299730	-1.185194	-1.398883
4	6	0	-0.067479	-1.608141	-1.342794
5	6	0	2.302923	-1.475794	-0.302285
6	6	0	1.754183	-0.355572	-2.395861
7	6	0	1.801977	-2.129133	1.002790
8	6	0	2.762734	-1.603197	2.082392
9	6	0	2.937044	-0.124909	1.702152
10	6	0	3.043186	-0.120476	0.151120
11	6	0	2.558727	1.120880	-0.550457
12	15	0	-2.192130	1.268991	1.767064
13	6	0	1.305572	1.676741	-0.336486
14	8	0	0.398631	1.183150	0.411776
15	8	0	1.067082	2.843038	-1.034139
16	6	0	-0.153205	3.513592	-0.766903
17	1	0	-3.046702	-2.670732	-1.395675
18	1	0	-3.861786	-2.163143	0.492636
19	1	0	-4.248718	-0.938596	-1.181422
20	1	0	-0.251892	-2.534892	-0.796844
21	1	0	-0.590757	-1.581760	-2.300210
22	1	0	3.079100	-2.128211	-0.726000
23	1	0	1.084093	0.033217	-3.159748
24	1	0	2.813115	-0.231917	-2.589390
25	1	0	1.778831	-3.224327	0.946180
26	1	0	0.784312	-1.785781	1.229548
27	1	0	3.724236	-2.133174	2.022152
28	1	0	2.378695	-1.742537	3.099993
29	1	0	2.049563	0.437557	2.004629
30	1	0	3.809853	0.342650	2.172193
31	1	0	4.101960	-0.236976	-0.109692
32	1	0	3.266508	1.721997	-1.111152
33	1	0	-1.290865	1.317716	2.855325
34	1	0	-2.274993	2.669631	1.571899
35	1	0	-3.374656	1.171538	2.554271
36	1	0	-0.244880	3.782963	0.292644
37	1	0	-1.023435	2.910561	-1.052279
38	1	0	-0.129137	4.423932	-1.371172

TS(7,5)*E*

Zero-point correction= 0.304828 (Hartree/Particle)
Thermal correction to Energy= 0.326218
Thermal correction to Enthalpy= 0.327162
Thermal correction to Gibbs Free Energy= 0.252850
Sum of electronic and zero-point Energies= -1391.939016
Sum of electronic and thermal Energies= -1391.917627
Sum of electronic and thermal Enthalpies= -1391.916683
Sum of electronic and thermal Free Energies= -1391.990994

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.412502	-0.442908	-0.035263
2	15	0	2.995201	-2.071620	0.400968
3	6	0	-1.384594	-1.102066	0.927758
4	6	0	-0.096229	-1.730486	0.912590
5	6	0	-2.242114	-1.082410	-0.313554
6	6	0	-1.812568	-0.333517	1.981161
7	6	0	-3.609130	-1.803846	-0.207946
8	6	0	-4.522699	-1.041188	-1.178679
9	6	0	-4.149163	0.425729	-0.917723
10	6	0	-2.612288	0.430539	-0.719359
11	6	0	-2.132227	1.466716	0.254699
12	15	0	2.790342	1.136319	-1.542570
13	6	0	-0.800969	1.849511	0.280338
14	8	0	0.110997	1.332476	-0.447140
15	8	0	-0.486707	2.841012	1.184611
16	6	0	0.851661	3.309822	1.178083
17	1	0	4.108862	-1.756727	1.221838
18	1	0	2.640830	-3.277699	1.059747
19	1	0	3.744114	-2.670987	-0.645208
20	1	0	-0.008782	-2.581733	0.232988
21	1	0	0.328897	-1.939872	1.896132
22	1	0	-1.682145	-1.533169	-1.141027
23	1	0	-1.180090	-0.154829	2.847886
24	1	0	-2.850387	-0.041818	2.087039
25	1	0	-4.002275	-1.714174	0.813412
26	1	0	-3.532078	-2.874484	-0.430676
27	1	0	-5.587748	-1.249705	-1.023965
28	1	0	-4.282864	-1.316497	-2.215342
29	1	0	-4.468124	1.103569	-1.717552
30	1	0	-4.642843	0.764961	0.004021
31	1	0	-2.122034	0.610375	-1.683595
32	1	0	-2.844775	2.063105	0.814819
33	1	0	2.029084	1.479219	-2.683242
34	1	0	3.047437	2.463543	-1.120305
35	1	0	4.027042	0.968505	-2.228771
36	1	0	1.129836	3.730375	0.203701
37	1	0	1.563380	2.515639	1.433154
38	1	0	0.894037	4.094934	1.937094

1*H*

Zero-point correction= 0.205016 (Hartree/Particle)
Thermal correction to Energy= 0.215467

```
 Thermal correction to Enthalpy=                  0.216412
 Thermal correction to Gibbs Free Energy=         0.168048
 Sum of electronic and zero-point Energies=           -351.088318
 Sum of electronic and thermal Energies=              -351.077866
 Sum of electronic and thermal Enthalpies=            -351.076922
 Sum of electronic and thermal Free Energies=         -351.125286

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        2.595701   -0.215136   -0.063028
    2          6             0        3.382239    1.018935    0.088516
    3          6             0        1.449679   -0.850500    0.135454
    4          6             0        3.975358   -0.243158   -0.565789
    5          6             0        0.227933   -0.241234    0.772943
    6          6             0       -0.986608   -0.208817   -0.174324
    7          6             0       -2.249249    0.373905    0.489027
    8          6             0       -3.422452    0.445996   -0.450225
    9          6             0       -4.582593   -0.191936   -0.286603
   10          1             0        3.746815    1.298338    1.076609
   11          1             0        3.165727    1.870843   -0.555466
   12          1             0        1.360077   -1.887229   -0.195305
   13          1             0        4.148682   -0.223417   -1.641426
   14          1             0        4.732085   -0.796513   -0.010308
   15          1             0        0.460905    0.775983    1.112313
   16          1             0       -0.043979   -0.818928    1.670391
   17          1             0       -1.204658   -1.224641   -0.531141
   18          1             0       -0.731647    0.381402   -1.065224
   19          1             0       -2.515950   -0.227017    1.368937
   20          1             0       -2.014960    1.384389    0.859090
   21          1             0       -3.281727    1.068337   -1.336280
   22          1             0       -5.391277   -0.105785   -1.007862
   23          1             0       -4.770135   -0.824085    0.579838
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TS(1,2)*H*

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Zero-point correction=                           0.256543 (Hartree/Particle)
 Thermal correction to Energy=                    0.276176
 Thermal correction to Enthalpy=                  0.277121
 Thermal correction to Gibbs Free Energy=         0.203083
 Sum of electronic and zero-point Energies=          -1164.089075
 Sum of electronic and thermal Energies=             -1164.069441
 Sum of electronic and thermal Enthalpies=           -1164.068497
 Sum of electronic and thermal Free Energies=        -1164.142535

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        2.117076   -1.447145   -0.697435
    2          6             0        3.287166   -0.573998   -1.065498
    3          6             0        4.404625   -0.590651   -0.004410
    4          6             0        5.624591    0.260950   -0.404591
    5          6             0        0.877828   -1.011806   -0.493196
    6          6             0       -0.447693   -1.506174   -0.129528
    7          6             0        0.093623    0.222633   -0.510071
    8          1             0        2.321503   -2.513246   -0.577244
    9          1             0        2.943493    0.456777   -1.221841
   10          1             0        3.711853   -0.911425   -2.024161
```

11	1	0	4.725630	-1.627979	0.169430
12	1	0	4.005415	-0.229035	0.951822
13	1	0	6.000461	-0.101536	-1.374412
14	1	0	5.313532	1.302730	-0.559936
15	1	0	-0.985501	-2.090317	-0.876201
16	1	0	-0.592884	-1.832760	0.899878
17	1	0	-0.117313	0.667848	-1.482038
18	1	0	0.269103	0.938699	0.292548
19	46	0	-2.193512	0.064106	0.022432
20	15	0	-2.945184	2.297549	-0.229262
21	15	0	-4.024716	-1.268517	0.718711
22	1	0	-2.129007	3.400673	-0.622305
23	1	0	-3.540986	2.992331	0.859809
24	1	0	-3.987895	2.607766	-1.145845
25	1	0	-3.965888	-2.671260	0.975506
26	1	0	-5.206962	-1.356184	-0.067748
27	1	0	-4.714037	-0.969748	1.926577
28	6	0	6.733230	0.209485	0.611404
29	6	0	7.211595	1.256369	1.285576
30	1	0	7.153838	-0.779746	0.803435
31	1	0	8.010670	1.152884	2.015051
32	1	0	6.822807	2.261219	1.130546

2*H*

Zero-point correction= 0.259155 (Hartree/Particle)
Thermal correction to Energy= 0.278259
Thermal correction to Enthalpy= 0.279204
Thermal correction to Gibbs Free Energy= 0.207435
Sum of electronic and zero-point Energies= -1164.116978
Sum of electronic and thermal Energies= -1164.097874
Sum of electronic and thermal Enthalpies= -1164.096930
Sum of electronic and thermal Free Energies= -1164.168698

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.286782	-1.380035	-0.821989
2	6	0	0.210032	-0.132969	-1.482046
3	6	0	0.983163	-1.930899	-0.262884
4	6	0	-1.544222	-1.766150	-0.546131
5	46	0	1.820862	0.007274	-0.110500
6	15	0	2.182306	2.351698	-0.460882
7	6	0	-2.799641	-1.059001	-0.982975
8	6	0	-3.542011	-0.354473	0.170978
9	6	0	-4.853403	0.322042	-0.274959
10	15	0	3.431105	-0.609914	1.552390
11	6	0	-5.548866	1.051383	0.841827
12	6	0	-6.769371	0.775380	1.304701
13	1	0	-0.457637	0.732007	-1.499508
14	1	0	0.684255	-0.293057	-2.457154
15	1	0	1.616617	-2.446609	-0.993995
16	1	0	0.912413	-2.488739	0.675200
17	1	0	-1.681276	-2.648659	0.082238
18	1	0	2.315470	2.788917	-1.800898
19	1	0	3.223122	3.161515	0.069977
20	1	0	1.119274	3.220497	-0.113535
21	1	0	-3.490417	-1.782133	-1.445649
22	1	0	-2.565422	-0.320416	-1.761431

23	1	0	-2.874581	0.393673	0.621432
24	1	0	-3.764260	-1.081620	0.963742
25	1	0	-4.621742	1.031275	-1.085452
26	1	0	-5.530228	-0.429703	-0.703099
27	1	0	2.919841	-1.073355	2.788862
28	1	0	4.467348	0.192162	2.103673
29	1	0	4.239440	-1.739629	1.278748
30	1	0	-4.978943	1.859123	1.306107
31	1	0	-7.213149	1.333960	2.124915
32	1	0	-7.374333	-0.022247	0.877056

2H´

Zero-point correction= 0.231328 (Hartree/Particle)
Thermal correction to Energy= 0.246927
Thermal correction to Enthalpy= 0.247872
Thermal correction to Gibbs Free Energy= 0.185281
Sum of electronic and zero-point Energies= -820.977758
Sum of electronic and thermal Energies= -820.962158
Sum of electronic and thermal Enthalpies= -820.961213
Sum of electronic and thermal Free Energies= -821.023804

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.673118	-0.425415	-0.274206
2	15	0	-3.059663	1.369980	0.570959
3	6	0	0.743733	-1.463644	0.129386
4	6	0	-0.091287	-0.670018	1.071548
5	6	0	2.075734	-1.534086	0.005947
6	6	0	-0.327469	-1.909416	-0.817863
7	6	0	2.509439	1.597813	-0.902415
8	6	0	1.453777	2.387461	-0.690339
9	6	0	3.098397	-0.954827	0.948550
10	6	0	4.134429	-0.017977	0.287478
11	6	0	3.668292	1.431779	0.044007
12	1	0	-3.465718	2.473436	-0.223985
13	1	0	-4.325052	1.146665	1.172747
14	1	0	-2.517394	2.136271	1.630413
15	1	0	0.262714	0.322380	1.358149
16	1	0	-0.550907	-1.222011	1.897286
17	1	0	2.476795	-2.086936	-0.846711
18	1	0	-0.092532	-1.838705	-1.885427
19	1	0	-0.808160	-2.859869	-0.557669
20	1	0	2.577681	1.048455	-1.842460
21	1	0	0.661608	2.495316	-1.426327
22	1	0	3.655814	-1.786615	1.407837
23	1	0	2.603060	-0.431044	1.776942
24	1	0	5.029477	0.025797	0.922620
25	1	0	4.460916	-0.459463	-0.665495
26	1	0	4.529395	1.987204	-0.361381
27	1	0	3.424964	1.906501	1.004708
28	1	0	1.345455	2.959486	0.230033

$2H_t$´

Zero-point correction= 0.231536 (Hartree/Particle)
Thermal correction to Energy= 0.247120

```
 Thermal correction to Enthalpy=                  0.248064
 Thermal correction to Gibbs Free Energy=         0.185313
 Sum of electronic and zero-point Energies=           -820.980577
 Sum of electronic and thermal Energies=              -820.964994
 Sum of electronic and thermal Enthalpies=            -820.964049
 Sum of electronic and thermal Free Energies=         -821.026800

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         46             0       -1.744057   -0.446006   -0.237729
    2         15             0       -2.996158    1.569229    0.248281
    3          6             0        0.633685   -1.518210    0.295602
    4          6             0       -0.112430   -0.486771    1.068839
    5          6             0        1.952700   -1.708261    0.156315
    6          6             0       -0.507012   -2.095129   -0.487763
    7          6             0        3.098966    2.075265   -0.090150
    8          6             0        1.900913    2.664473   -0.096755
    9          6             0        3.041778   -0.967203    0.888008
   10          6             0        4.063494   -0.286759   -0.047006
   11          6             0        3.486425    0.864557   -0.896300
   12          1             0       -3.292818    2.553286   -0.730191
   13          1             0       -4.288208    1.545670    0.833963
   14          1             0       -2.415608    2.454971    1.187202
   15          1             0        0.308345    0.518754    1.132851
   16          1             0       -0.561937   -0.825310    2.007826
   17          1             0        2.283725   -2.467961   -0.555747
   18          1             0       -0.323112   -2.274398   -1.552548
   19          1             0       -1.020611   -2.935572   -0.006125
   20          1             0        3.888076    2.495400    0.538099
   21          1             0        1.083987    2.284708   -0.707973
   22          1             0        1.695317    3.551204    0.498090
   23          1             0        3.594541   -1.673373    1.527451
   24          1             0        2.604359   -0.219707    1.560850
   25          1             0        4.903347    0.092718    0.552763
   26          1             0        4.486982   -1.042087   -0.723510
   27          1             0        2.620773    0.504975   -1.466030
   28          1             0        4.250731    1.162807   -1.630372
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TS(2,3)*H*

```
Zero-point correction=                           0.258436 (Hartree/Particle)
 Thermal correction to Energy=                    0.276747
 Thermal correction to Enthalpy=                  0.277691
 Thermal correction to Gibbs Free Energy=         0.209713
 Sum of electronic and zero-point Energies=          -1164.084481
 Sum of electronic and thermal Energies=             -1164.066169
 Sum of electronic and thermal Enthalpies=           -1164.065225
 Sum of electronic and thermal Free Energies=        -1164.133203

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0       -0.464337   -1.836794    0.319321
    2          6             0       -0.765696   -1.749688    1.711852
    3          6             0       -1.608699   -2.048802   -0.538845
    4          6             0        0.691129   -1.310610   -0.329249
    5         46             0       -1.554677    0.021558    0.017742
```

6	15	0	-0.697884	1.968216	1.051500
7	6	0	1.939184	-0.949957	0.420682
8	6	0	2.992478	-0.242857	-0.443393
9	6	0	4.292392	0.075037	0.319744
10	15	0	-3.406415	0.699939	-1.155888
11	6	0	5.296927	0.822740	-0.514362
12	6	0	6.521476	0.391839	-0.821293
13	1	0	0.009596	-1.522106	2.434861
14	1	0	-1.664792	-2.223504	2.088453
15	1	0	-2.490211	-2.539468	-0.131663
16	1	0	-1.451942	-2.181373	-1.607339
17	1	0	0.778691	-1.487004	-1.398339
18	1	0	-1.225675	2.437362	2.279565
19	1	0	-0.676394	3.231416	0.404880
20	1	0	0.660376	1.950773	1.450095
21	1	0	2.395716	-1.855353	0.867857
22	1	0	1.696754	-0.310490	1.286592
23	1	0	2.563999	0.686485	-0.845433
24	1	0	3.233862	-0.868155	-1.313939
25	1	0	4.038787	0.675710	1.207954
26	1	0	4.740557	-0.855893	0.691927
27	1	0	-3.528782	0.383236	-2.533425
28	1	0	-3.715261	2.077465	-1.281231
29	1	0	-4.714911	0.280546	-0.796167
30	1	0	4.965871	1.789553	-0.899695
31	1	0	7.198788	0.977455	-1.437657
32	1	0	6.895473	-0.566105	-0.464324

TS(2,3)*H´*

Zero-point correction= 0.232590 (Hartree/Particle)
Thermal correction to Energy= 0.246294
Thermal correction to Enthalpy= 0.247238
Thermal correction to Gibbs Free Energy= 0.192632
Sum of electronic and zero-point Energies= -820.958218
Sum of electronic and thermal Energies= -820.944515
Sum of electronic and thermal Enthalpies= -820.943571
Sum of electronic and thermal Free Energies= -820.998177

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.641361	-1.823679	0.066803
2	6	0	-0.708770	-2.166507	-0.332661
3	6	0	0.762029	-1.631062	1.481461
4	6	0	1.467327	-1.258539	-0.936270
5	46	0	-0.632849	-0.075027	0.141628
6	6	0	2.810402	-0.646941	-0.674976
7	15	0	-2.775661	0.497041	-0.457887
8	6	0	0.103504	1.859076	1.191569
9	6	0	0.556581	1.986604	-0.103017
10	6	0	1.987918	1.826659	-0.572159
11	6	0	2.854301	0.723887	0.061632
12	1	0	-0.927511	-2.333374	-1.385750
13	1	0	-1.339856	-2.711559	0.365412
14	1	0	0.132211	-2.218201	2.141079
15	1	0	1.676912	-1.238715	1.911567
16	1	0	1.179303	-1.438720	-1.967297
17	1	0	3.331092	-0.521696	-1.633312

18	1	0	3.432156	-1.336271	-0.076448
19	1	0	-3.898845	-0.007227	0.248469
20	1	0	-3.167191	1.860734	-0.417712
21	1	0	-3.292699	0.223943	-1.752619
22	1	0	-0.834132	2.311888	1.498404
23	1	0	0.752129	1.523408	1.993582
24	1	0	-0.091587	2.499055	-0.812582
25	1	0	1.992940	1.713509	-1.662868
26	1	0	2.471450	2.797178	-0.370022
27	1	0	3.900274	1.058854	0.064700
28	1	0	2.581420	0.595799	1.114523

TS(2,3)H_t'

Zero-point correction= 0.232191 (Hartree/Particle)
Thermal correction to Energy= 0.246141
Thermal correction to Enthalpy= 0.247085
Thermal correction to Gibbs Free Energy= 0.191507
Sum of electronic and zero-point Energies= -820.954218
Sum of electronic and thermal Energies= -820.940268
Sum of electronic and thermal Enthalpies= -820.939324
Sum of electronic and thermal Free Energies= -820.994902

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.562849	1.848138	0.066604
2	6	0	0.746150	2.089244	-0.501415
3	6	0	-0.552332	1.843476	1.500332
4	6	0	-1.498119	1.226754	-0.809880
5	46	0	0.657557	0.055634	0.161738
6	6	0	-2.815536	0.666332	-0.373950
7	15	0	2.727176	-0.570577	-0.606614
8	6	0	0.170318	-2.072422	1.025584
9	6	0	-1.059207	-1.515707	0.785823
10	6	0	-1.913470	-1.816168	-0.424953
11	6	0	-3.065760	-0.826270	-0.725951
12	1	0	0.858310	2.141961	-1.582687
13	1	0	1.472774	2.660260	0.072006
14	1	0	0.180833	2.456617	2.012051
15	1	0	-1.440139	1.584085	2.067233
16	1	0	-1.302375	1.303073	-1.876703
17	1	0	-3.654352	1.232378	-0.814971
18	1	0	-2.922559	0.791670	0.709654
19	1	0	3.910158	-0.198714	0.085769
20	1	0	3.066530	-1.938733	-0.761332
21	1	0	3.173471	-0.145845	-1.885307
22	1	0	0.605487	-2.783091	0.326538
23	1	0	0.624897	-2.015105	2.009562
24	1	0	-1.525311	-0.964510	1.600355
25	1	0	-1.256381	-1.916064	-1.294876
26	1	0	-2.367237	-2.809036	-0.273490
27	1	0	-3.302726	-0.912652	-1.794210
28	1	0	-3.971802	-1.147079	-0.193482

3*H*

Zero-point correction= 0.258964 (Hartree/Particle)

```
 Thermal correction to Energy=                  0.278173
 Thermal correction to Enthalpy=                0.279118
 Thermal correction to Gibbs Free Energy=       0.207855
 Sum of electronic and zero-point Energies=         -1164.113263
 Sum of electronic and thermal Energies=            -1164.094054
 Sum of electronic and thermal Enthalpies=          -1164.093110
 Sum of electronic and thermal Free Energies=       -1164.164373

 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1          6             0        0.634031   -2.642486    1.607679
    2          6             0        0.264165   -1.748792    0.677334
    3          6             0       -0.755903   -1.897875   -0.398306
    4          6             0        0.516096   -0.270156    0.670834
    5          6             0        1.566427    0.242745   -0.316808
    6          6             0        3.001698   -0.117099    0.117038
    7          6             0        4.067908    0.342231   -0.897051
    8          6             0        5.464883   -0.042562   -0.492670
    9          6             0        6.464362    0.809132   -0.257086
   10         46             0       -1.477716    0.061592   -0.016506
   11         15             0       -1.595558    2.317290    0.770899
   12         15             0       -3.646151   -0.352936   -0.965092
   13          1             0        0.268518   -3.667199    1.588979
   14          1             0        1.282302   -2.364199    2.435701
   15          1             0       -0.362774   -1.840383   -1.418803
   16          1             0       -1.472454   -2.716379   -0.289292
   17          1             0        0.662508    0.155019    1.671390
   18          1             0        1.490498    1.334238   -0.425290
   19          1             0        1.382992   -0.178721   -1.314436
   20          1             0        3.069342   -1.203830    0.258899
   21          1             0        3.215940    0.337036    1.094429
   22          1             0        3.834676   -0.108107   -1.874774
   23          1             0        4.009168    1.430952   -1.032627
   24          1             0        5.644020   -1.113170   -0.374795
   25          1             0        6.333236    1.885171   -0.357915
   26          1             0        7.451806    0.467253    0.042345
   27          1             0       -0.409400    3.089262    0.727444
   28          1             0       -1.863687    2.514729    2.148166
   29          1             0       -2.463003    3.338369    0.297983
   30          1             0       -4.446732   -1.321741   -0.312389
   31          1             0       -3.670962   -0.959540   -2.243980
   32          1             0       -4.697415    0.571885   -1.214655
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3*H´*

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Zero-point correction=                          0.232974 (Hartree/Particle)
 Thermal correction to Energy=                  0.247439
 Thermal correction to Enthalpy=                0.248383
 Thermal correction to Gibbs Free Energy=       0.190810
 Sum of electronic and zero-point Energies=          -820.993557
 Sum of electronic and thermal Energies=             -820.979093
 Sum of electronic and thermal Enthalpies=           -820.978148
 Sum of electronic and thermal Free Energies=        -821.035721

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

1	46	0	0.536060	-0.028801	-0.087835
2	15	0	2.901729	0.006773	0.285890
3	6	0	-0.948473	2.164452	-0.102946
4	6	0	0.315247	1.940414	0.648885
5	6	0	-1.441011	0.764805	-0.314889
6	6	0	-1.386972	3.282235	-0.696875
7	6	0	-0.630672	-2.008481	-0.716694
8	6	0	0.698944	-2.326115	-0.650487
9	6	0	-2.401252	0.180420	0.715103
10	6	0	-2.806563	-1.270879	0.420712
11	6	0	-1.641016	-2.274876	0.375075
12	1	0	3.776592	-1.089952	0.517322
13	1	0	3.676851	0.607522	-0.736647
14	1	0	3.379024	0.815789	1.344835
15	1	0	0.186358	1.765836	1.723599
16	1	0	1.132003	2.642347	0.456278
17	1	0	-1.799681	0.593075	-1.336851
18	1	0	-2.265487	3.277294	-1.339075
19	1	0	-0.863095	4.229524	-0.585255
20	1	0	-1.044919	-1.748251	-1.689706
21	1	0	1.313797	-2.347432	-1.545902
22	1	0	-3.317578	0.795377	0.731493
23	1	0	-1.975080	0.253471	1.725447
24	1	0	-3.530708	-1.610502	1.172382
25	1	0	-3.332372	-1.302307	-0.545542
26	1	0	-2.062478	-3.277810	0.201328
27	1	0	-1.132459	-2.317785	1.347305
28	1	0	1.125175	-2.774803	0.243722

3H_t´

Zero-point correction= 0.232651 (Hartree/Particle)
Thermal correction to Energy= 0.247415
Thermal correction to Enthalpy= 0.248360
Thermal correction to Gibbs Free Energy= 0.190440
Sum of electronic and zero-point Energies= -820.987769
Sum of electronic and thermal Energies= -820.973005
Sum of electronic and thermal Enthalpies= -820.972061
Sum of electronic and thermal Free Energies= -821.029980

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.522434	-0.002116	0.056421
2	15	0	-2.912740	-0.061275	-0.360410
3	6	0	0.974193	2.134242	0.183564
4	6	0	-0.235136	1.966229	-0.672256
5	6	0	1.438199	0.714323	0.319362
6	6	0	1.364824	3.201951	0.893207
7	6	0	0.356582	-2.247283	0.222480
8	6	0	-0.392721	-2.045498	1.342471
9	6	0	2.428792	0.199132	-0.724234
10	6	0	2.378923	-1.319036	-1.029309
11	6	0	1.862300	-2.193343	0.132116
12	1	0	-3.834058	-1.141411	-0.248665
13	1	0	-3.686059	0.865202	0.381289
14	1	0	-3.343649	0.367460	-1.639354
15	1	0	-0.024988	1.826699	-1.738173
16	1	0	-1.056836	2.670221	-0.514546

17	1	0	1.736966	0.448151	1.340229
18	1	0	2.192321	3.144903	1.597346
19	1	0	0.850352	4.157358	0.812960
20	1	0	-0.137449	-2.659053	-0.659286
21	1	0	0.066007	-1.745909	2.281621
22	1	0	-1.437007	-2.337990	1.385351
23	1	0	3.441565	0.456386	-0.372076
24	1	0	2.295443	0.752026	-1.661940
25	1	0	1.730332	-1.493572	-1.899056
26	1	0	3.379256	-1.662229	-1.322225
27	1	0	2.289719	-1.868787	1.088300
28	1	0	2.205416	-3.227273	-0.025377

TS(3,4)*H*´

Zero-point correction= 0.233801 (Hartree/Particle)
Thermal correction to Energy= 0.247004
Thermal correction to Enthalpy= 0.247948
Thermal correction to Gibbs Free Energy= 0.193230
Sum of electronic and zero-point Energies= -820.952287
Sum of electronic and thermal Energies= -820.939084
Sum of electronic and thermal Enthalpies= -820.938140
Sum of electronic and thermal Free Energies= -820.992858

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.757397	-0.070649	0.073796
2	15	0	-2.845015	-0.662680	-0.437323
3	6	0	0.539847	1.879740	0.128147
4	6	0	-0.448537	1.786823	-0.961284
5	6	0	1.587565	0.769888	0.190279
6	6	0	0.432316	2.745203	1.174570
7	6	0	1.371865	-1.037039	0.916405
8	6	0	0.044754	-1.627059	1.229485
9	6	0	2.386126	0.453466	-1.070957
10	6	0	3.202565	-0.809629	-0.776907
11	6	0	2.224784	-1.783085	-0.109656
12	1	0	-3.401681	-1.915248	-0.073066
13	1	0	-3.883089	0.152021	0.072284
14	1	0	-3.266137	-0.673670	-1.789055
15	1	0	-0.071653	1.564802	-1.960223
16	1	0	-1.206412	2.570788	-0.968417
17	1	0	2.270603	1.036390	0.997173
18	1	0	1.104553	2.699760	2.027135
19	1	0	-0.327314	3.521613	1.183532
20	1	0	1.920861	-0.790225	1.826589
21	1	0	-0.254433	-1.597845	2.277649
22	1	0	3.031195	1.303330	-1.332011
23	1	0	1.718920	0.280882	-1.923407
24	1	0	3.658124	-1.234853	-1.678402
25	1	0	4.021635	-0.567441	-0.084986
26	1	0	2.746412	-2.618604	0.375564
27	1	0	1.560141	-2.217778	-0.868473
28	1	0	-0.153966	-2.593714	0.762844

TS(3,4)H_t´

Zero-point correction= 0.233217 (Hartree/Particle)
Thermal correction to Energy= 0.246672
Thermal correction to Enthalpy= 0.247616
Thermal correction to Gibbs Free Energy= 0.192295
Sum of electronic and zero-point Energies= -820.940576
Sum of electronic and thermal Energies= -820.927121
Sum of electronic and thermal Enthalpies= -820.926176
Sum of electronic and thermal Free Energies= -820.981498

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.809019	-0.158924	-0.020636
2	15	0	-3.034119	-0.469957	-0.119762
3	6	0	0.477352	1.847530	0.154796
4	6	0	-0.542849	1.783785	-0.902082
5	6	0	1.423705	0.641508	0.210093
6	6	0	0.502213	2.741382	1.174372
7	6	0	1.219197	-1.352680	-0.045742
8	6	0	0.109114	-1.963609	0.685927
9	6	0	2.628766	0.713499	-0.720464
10	6	0	3.528029	-0.519240	-0.451348
11	6	0	2.682247	-1.532630	0.348535
12	1	0	-3.675035	-1.681516	0.245805
13	1	0	-3.838583	0.397064	0.656468
14	1	0	-3.706397	-0.287761	-1.352229
15	1	0	-0.184931	1.585231	-1.915798
16	1	0	-1.308174	2.559646	-0.872877
17	1	0	1.748437	0.534579	1.246927
18	1	0	1.183871	2.637504	2.014506
19	1	0	-0.168101	3.596913	1.183048
20	1	0	1.126999	-1.483618	-1.129163
21	1	0	0.234053	-2.086412	1.762725
22	1	0	-0.379374	-2.809228	0.202598
23	1	0	3.158190	1.655998	-0.528287
24	1	0	2.298886	0.753308	-1.765801
25	1	0	3.867798	-0.964584	-1.393101
26	1	0	4.428184	-0.240282	0.106584
27	1	0	2.800491	-1.396342	1.430113
28	1	0	2.973687	-2.567888	0.129675

4*H*´

Zero-point correction= 0.236109 (Hartree/Particle)
Thermal correction to Energy= 0.249679
Thermal correction to Enthalpy= 0.250623
Thermal correction to Gibbs Free Energy= 0.194472
Sum of electronic and zero-point Energies= -821.007386
Sum of electronic and thermal Energies= -820.993816
Sum of electronic and thermal Enthalpies= -820.992871
Sum of electronic and thermal Free Energies= -821.049022

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.253992	-0.497673	0.062743
2	15	0	3.130372	0.930204	-0.495973
3	6	0	-1.560650	-1.318374	-0.113433

4	6	0	-2.063327	-1.787015	-1.270345
5	6	0	-2.220281	-0.224124	0.717534
6	6	0	-0.287230	-1.822563	0.450534
7	6	0	-1.280134	1.003667	0.891472
8	6	0	0.150334	0.741240	1.326528
9	6	0	-3.475175	0.435946	0.111886
10	6	0	-2.948300	1.553265	-0.833800
11	6	0	-1.461687	1.768227	-0.437297
12	1	0	3.180875	2.194319	0.140944
13	1	0	4.471343	0.560462	-0.216579
14	1	0	3.376988	1.407484	-1.809236
15	1	0	-2.970333	-1.399481	-1.722692
16	1	0	-1.567504	-2.592108	-1.808086
17	1	0	-2.443350	-0.659320	1.703416
18	1	0	-0.337093	-2.016627	1.527133
19	1	0	0.086689	-2.717417	-0.070938
20	1	0	-1.736853	1.619970	1.687904
21	1	0	0.200325	0.275893	2.315748
22	1	0	-4.057768	0.883273	0.926394
23	1	0	-4.138550	-0.275222	-0.388884
24	1	0	-3.030651	1.256571	-1.884549
25	1	0	-3.535907	2.471070	-0.719300
26	1	0	-1.194862	2.827287	-0.340810
27	1	0	-0.795297	1.331859	-1.191114
28	1	0	0.731408	1.670284	1.345610

4H_t

Zero-point correction= 0.235683 (Hartree/Particle)
Thermal correction to Energy= 0.249600
Thermal correction to Enthalpy= 0.250545
Thermal correction to Gibbs Free Energy= 0.193005
Sum of electronic and zero-point Energies= -821.009677
Sum of electronic and thermal Energies= -820.995760
Sum of electronic and thermal Enthalpies= -820.994816
Sum of electronic and thermal Free Energies= -821.052356

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.388195	0.387902	-0.179579
2	15	0	3.250662	-0.979153	0.569348
3	6	0	-1.351394	1.576387	0.010119
4	6	0	-1.746093	2.484542	0.920213
5	6	0	-2.116300	0.307268	-0.288095
6	6	0	-0.097992	1.706905	-0.772998
7	6	0	-3.469534	0.045935	0.390824
8	6	0	-3.713374	-1.478156	0.201707
9	6	0	-2.328441	-2.092685	-0.162144
10	6	0	-1.302894	-0.956152	0.083269
11	6	0	0.011765	-1.109978	-0.651255
12	1	0	3.020656	-2.371901	0.688425
13	1	0	4.458908	-1.082341	-0.167037
14	1	0	3.862591	-0.813315	1.838778
15	1	0	-2.660521	2.375689	1.495069
16	1	0	-1.160062	3.381048	1.110112
17	1	0	-2.270679	0.267063	-1.381123
18	1	0	-0.257003	1.556767	-1.847065
19	1	0	0.407208	2.671981	-0.609095
20	1	0	-4.278455	0.659452	-0.019700

21	1	0	-3.395758	0.281786	1.459412
22	1	0	-4.439950	-1.665934	-0.596572
23	1	0	-4.127679	-1.926814	1.111008
24	1	0	-2.095889	-2.992397	0.418208
25	1	0	-2.303572	-2.381033	-1.221225
26	1	0	-1.105605	-0.903321	1.164969
27	1	0	0.530513	-2.034266	-0.374436
28	1	0	-0.116067	-1.083042	-1.739137

4*H*

Zero-point correction= 0.264106 (Hartree/Particle)
Thermal correction to Energy= 0.281098
Thermal correction to Enthalpy= 0.282042
Thermal correction to Gibbs Free Energy= 0.218242
Sum of electronic and zero-point Energies= -1164.138643
Sum of electronic and thermal Energies= -1164.121651
Sum of electronic and thermal Enthalpies= -1164.120707
Sum of electronic and thermal Free Energies= -1164.184508

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.022460	-0.129543	-0.211950
2	15	0	-2.884012	1.403524	-0.098782
3	6	0	1.222262	1.707821	0.339818
4	6	0	0.244996	1.487286	-0.757869
5	6	0	2.315138	0.676015	0.526413
6	6	0	1.155028	2.775839	1.157338
7	6	0	3.386815	0.647309	-0.606957
8	6	0	3.921806	-0.812684	-0.655759
9	6	0	3.171557	-1.565983	0.468754
10	6	0	1.837334	-0.797920	0.641034
11	6	0	0.790420	-1.206376	-0.398700
12	15	0	-2.125324	-2.169187	0.412192
13	1	0	-2.704235	2.551455	0.710285
14	1	0	-3.243390	2.095228	-1.282115
15	1	0	-4.210486	1.116360	0.321809
16	1	0	0.708290	1.180717	-1.699210
17	1	0	-0.352229	2.386477	-0.944490
18	1	0	2.841866	0.911164	1.461130
19	1	0	1.855848	2.914935	1.977027
20	1	0	0.399608	3.548996	1.029653
21	1	0	4.178297	1.376426	-0.403272
22	1	0	2.945326	0.929980	-1.568306
23	1	0	5.008152	-0.863026	-0.523384
24	1	0	3.704399	-1.266588	-1.629188
25	1	0	3.024879	-2.629248	0.244180
26	1	0	3.744562	-1.509304	1.404855
27	1	0	1.423970	-0.973258	1.643700
28	1	0	0.584853	-2.280931	-0.295104
29	1	0	-2.148500	-3.205127	-0.553709
30	1	0	-1.535015	-2.931006	1.449915
31	1	0	-3.470190	-2.325316	0.844018
32	1	0	1.145050	-1.051851	-1.423697

4H_t

Zero-point correction=	0.263672 (Hartree/Particle)
Thermal correction to Energy=	0.280773
Thermal correction to Enthalpy=	0.281717
Thermal correction to Gibbs Free Energy=	0.217629
Sum of electronic and zero-point Energies=	-1164.140051
Sum of electronic and thermal Energies=	-1164.122951
Sum of electronic and thermal Enthalpies=	-1164.122007
Sum of electronic and thermal Free Energies=	-1164.186094

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.112958	-0.108519	0.216650
2	15	0	-2.201558	-2.124002	-0.504065
3	6	0	1.321210	1.664641	0.093153
4	6	0	1.495614	2.692990	-0.756493
5	6	0	2.350005	0.576849	0.296082
6	6	0	0.093015	1.508431	0.918616
7	6	0	3.692268	0.646667	-0.448973
8	6	0	4.282752	-0.786932	-0.322205
9	6	0	3.092491	-1.703164	0.090431
10	6	0	1.826176	-0.829340	-0.080006
11	6	0	0.595962	-1.275872	0.694504
12	15	0	-2.868857	1.482575	-0.237252
13	1	0	-1.535574	-2.903928	-1.480853
14	1	0	-2.342898	-3.155497	0.456210
15	1	0	-3.502864	-2.245554	-1.062292
16	1	0	2.392430	2.810472	-1.356622
17	1	0	0.736702	3.464976	-0.869509
18	1	0	2.568814	0.542505	1.378510
19	1	0	0.320687	1.236406	1.954694
20	1	0	-0.499982	2.429886	0.925178
21	1	0	4.361270	1.418157	-0.052575
22	1	0	3.515096	0.885113	-1.504963
23	1	0	5.078331	-0.821098	0.430511
24	1	0	4.734412	-1.110771	-1.266315
25	1	0	3.042371	-2.626392	-0.498383
26	1	0	3.185177	-2.001931	1.143201
27	1	0	1.583032	-0.799139	-1.154872
28	1	0	0.381498	-2.332751	0.483000
29	1	0	0.753809	-1.189289	1.777001
30	1	0	-4.154491	1.210722	-0.777684
31	1	0	-3.316469	2.291749	0.835918
32	1	0	-2.546003	2.544010	-1.116931

TS(4,5)*H*

Zero-point correction=	0.261329 (Hartree/Particle)
Thermal correction to Energy=	0.278700
Thermal correction to Enthalpy=	0.279644
Thermal correction to Gibbs Free Energy=	0.213234
Sum of electronic and zero-point Energies=	-1164.104152
Sum of electronic and thermal Energies=	-1164.086782
Sum of electronic and thermal Enthalpies=	-1164.085838
Sum of electronic and thermal Free Energies=	-1164.152247

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

1	46	0	-1.228621	-0.011045	0.035967
2	15	0	-1.254783	2.336567	-0.436530
3	15	0	-3.364478	-1.109833	-0.085656
4	1	0	-2.212567	3.250462	0.085450
5	1	0	-0.143497	3.190125	-0.184155
6	1	0	-1.424470	2.757852	-1.783160
7	1	0	-3.531454	-2.518579	-0.220967
8	1	0	-4.194972	-1.008956	1.062919
9	1	0	-4.408124	-0.797823	-1.002101
10	6	0	1.753961	0.044258	1.380162
11	6	0	2.125959	1.224445	1.896117
12	6	0	2.645729	-0.889104	0.583065
13	6	0	0.381418	-0.498603	1.516598
14	6	0	3.941424	-0.306777	-0.005369
15	6	0	3.521562	0.394518	-1.327879
16	6	0	2.091712	-0.121065	-1.647731
17	6	0	1.824868	-1.287016	-0.668809
18	6	0	0.353145	-1.556292	-0.381045
19	1	0	3.130862	1.620310	1.782832
20	1	0	1.428996	1.836231	2.464115
21	1	0	2.850737	-1.772339	1.207139
22	1	0	-0.283111	0.158313	2.099490
23	1	0	0.363816	-1.492156	1.966460
24	1	0	4.628637	-1.133805	-0.221782
25	1	0	4.469431	0.360162	0.683617
26	1	0	4.226939	0.160863	-2.132893
27	1	0	3.524291	1.483719	-1.216393
28	1	0	1.351460	0.667119	-1.466304
29	1	0	1.975977	-0.433448	-2.691785
30	1	0	2.260505	-2.206507	-1.091944
31	1	0	0.177381	-2.524729	0.087510
32	1	0	-0.224018	-1.515942	-1.320390

TS(4,5)H_t

Zero-point correction= 0.261051 (Hartree/Particle)
Thermal correction to Energy= 0.278656
Thermal correction to Enthalpy= 0.279600
Thermal correction to Gibbs Free Energy= 0.211246
Sum of electronic and zero-point Energies= -1164.101767
Sum of electronic and thermal Energies= -1164.084163
Sum of electronic and thermal Enthalpies= -1164.083218
Sum of electronic and thermal Free Energies= -1164.151572

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.336820	-0.048551	-0.056471
2	15	0	-1.499279	2.080331	-1.126503
3	15	0	-3.364208	-1.254514	0.322437
4	1	0	-2.111669	3.155175	-0.427036
5	1	0	-0.387171	2.856881	-1.561758
6	1	0	-2.243144	2.288914	-2.320943
7	1	0	-3.498515	-2.357020	1.215349
8	1	0	-4.582461	-0.645345	0.734471
9	1	0	-3.951425	-1.936234	-0.777969
10	6	0	1.535279	0.429564	1.525925
11	6	0	1.692714	1.613218	2.134854

12	6	0	2.569693	-0.270006	0.693690
13	6	0	0.257456	-0.335330	1.523802
14	6	0	3.920525	0.335995	0.303535
15	6	0	4.309766	-0.445472	-0.995616
16	6	0	3.022291	-1.197890	-1.466304
17	6	0	1.892254	-0.524874	-0.663684
18	6	0	0.564498	-1.214092	-0.465433
19	1	0	2.641193	2.143242	2.121350
20	1	0	0.878082	2.085942	2.678745
21	1	0	2.753976	-1.260816	1.146922
22	1	0	-0.547383	0.191966	2.060052
23	1	0	0.359531	-1.337140	1.941810
24	1	0	4.679308	0.247323	1.087999
25	1	0	3.802037	1.404326	0.084554
26	1	0	5.125076	-1.151472	-0.804922
27	1	0	4.668488	0.242708	-1.768323
28	1	0	2.873479	-1.140900	-2.549912
29	1	0	3.080588	-2.262143	-1.202639
30	1	0	1.695903	0.461184	-1.112033
31	1	0	-0.028998	-1.273244	-1.393693
32	1	0	0.652274	-2.213933	-0.037978

TS(4,5)*H´*

Zero-point correction= 0.235553 (Hartree/Particle)
Thermal correction to Energy= 0.248841
Thermal correction to Enthalpy= 0.249786
Thermal correction to Gibbs Free Energy= 0.193254
Sum of electronic and zero-point Energies= -820.988447
Sum of electronic and thermal Energies= -820.975159
Sum of electronic and thermal Enthalpies= -820.974214
Sum of electronic and thermal Free Energies= -821.030746

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.368060	0.222189	0.190865
2	15	0	-3.339753	-0.627714	-0.656134
3	1	0	-4.398989	-1.021404	0.201115
4	1	0	-4.148020	0.144229	-1.530884
5	1	0	-3.356140	-1.801736	-1.452170
6	6	0	1.571223	1.319855	-0.215802
7	6	0	1.763929	1.860442	-1.425890
8	6	0	2.544451	0.411464	0.511196
9	6	0	0.325369	1.531096	0.570516
10	6	0	3.638398	-0.269954	-0.325435
11	6	0	2.947423	-1.491957	-0.990123
12	6	0	1.645217	-1.741342	-0.178275
13	6	0	1.693023	-0.774916	1.030082
14	6	0	0.333135	-0.339963	1.552231
15	1	0	2.671228	1.694058	-1.999412
16	1	0	1.013273	2.498577	-1.885444
17	1	0	2.972729	0.976073	1.353507
18	1	0	-0.412826	2.157314	0.026013
19	1	0	0.497938	1.997136	1.541237
20	1	0	4.432934	-0.608981	0.350792
21	1	0	4.113034	0.399486	-1.050057
22	1	0	3.607875	-2.365906	-0.985761
23	1	0	2.710306	-1.282960	-2.038213

24	1	0	0.762046	-1.506014	-0.785203
25	1	0	1.541150	-2.782902	0.145357
26	1	0	2.236284	-1.262571	1.854445
27	1	0	0.370218	0.127763	2.535105
28	1	0	-0.359002	-1.195500	1.610815

TS(4,5)H_t'

Zero-point correction= 0.235173 (Hartree/Particle)
Thermal correction to Energy= 0.248664
Thermal correction to Enthalpy= 0.249608
Thermal correction to Gibbs Free Energy= 0.192410
Sum of electronic and zero-point Energies= -820.984502
Sum of electronic and thermal Energies= -820.971011
Sum of electronic and thermal Enthalpies= -820.970067
Sum of electronic and thermal Free Energies= -821.027265

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.501332	-0.214656	0.183460
2	15	0	-3.619748	-0.106308	-0.694659
3	1	0	-4.702956	0.402359	0.067354
4	1	0	-3.893266	0.657775	-1.858378
5	1	0	-4.297088	-1.273954	-1.133962
6	6	0	1.295756	1.551562	0.279946
7	6	0	1.311869	2.706677	-0.395469
8	6	0	2.386790	0.522052	0.297809
9	6	0	0.129713	1.070921	1.084703
10	6	0	3.615763	0.532235	-0.614945
11	6	0	4.037255	-0.975513	-0.673314
12	6	0	2.851436	-1.796361	-0.067448
13	6	0	1.684920	-0.794005	-0.071642
14	6	0	0.472095	-0.983150	0.812259
15	1	0	2.185328	3.026526	-0.957428
16	1	0	0.454561	3.375522	-0.403740
17	1	0	2.731709	0.414011	1.342374
18	1	0	-0.743618	1.735323	0.992520
19	1	0	0.360221	0.962999	2.144937
20	1	0	4.422329	1.177188	-0.251215
21	1	0	3.336629	0.890775	-1.613298
22	1	0	4.960421	-1.152841	-0.111511
23	1	0	4.237771	-1.280096	-1.705891
24	1	0	2.639424	-2.709771	-0.633144
25	1	0	3.078759	-2.097628	0.963688
26	1	0	1.329891	-0.687688	-1.108188
27	1	0	-0.167034	-1.828737	0.471848
28	1	0	0.710845	-1.149470	1.863341

5H

Zero-point correction= 0.210721 (Hartree/Particle)
Thermal correction to Energy= 0.218770
Thermal correction to Enthalpy= 0.219714
Thermal correction to Gibbs Free Energy= 0.176962
Sum of electronic and zero-point Energies= -351.154990
Sum of electronic and thermal Energies= -351.146941
Sum of electronic and thermal Enthalpies= -351.145997

Sum of electronic and thermal Free Energies= -351.188749

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.460225	-0.436442	0.122637
2	6	0	2.235752	-1.468730	-0.213675
3	6	0	0.015983	-0.514332	0.596572
4	6	0	1.841127	1.029568	0.031017
5	6	0	-0.950488	-1.419585	-0.202855
6	6	0	-2.306694	-0.706308	-0.069299
7	6	0	-1.946976	0.785938	-0.226433
8	6	0	-0.560572	0.940312	0.450050
9	6	0	0.515227	1.721886	-0.341078
10	1	0	1.888032	-2.496637	-0.140480
11	1	0	3.252633	-1.326545	-0.572468
12	1	0	-0.011510	-0.819553	1.651822
13	1	0	2.655325	1.219605	-0.676870
14	1	0	2.178737	1.387646	1.016380
15	1	0	-0.967402	-2.453063	0.160519
16	1	0	-0.643156	-1.448923	-1.256178
17	1	0	-2.727271	-0.889775	0.929067
18	1	0	-3.048054	-1.047605	-0.801090
19	1	0	-1.870821	1.032834	-1.293813
20	1	0	-2.706089	1.450884	0.200031
21	1	0	-0.673138	1.392792	1.442670
22	1	0	0.336549	1.608946	-1.418846
23	1	0	0.514666	2.795551	-0.122360

5 H_t

Zero-point correction= 0.210542 (Hartree/Particle)
Thermal correction to Energy= 0.218700
Thermal correction to Enthalpy= 0.219644
Thermal correction to Gibbs Free Energy= 0.177674
Sum of electronic and zero-point Energies= -351.143449
Sum of electronic and thermal Energies= -351.135291
Sum of electronic and thermal Enthalpies= -351.134347
Sum of electronic and thermal Free Energies= -351.176317

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.460502	-0.498490	0.088566
2	6	0	2.216679	-1.576580	-0.119111
3	6	0	-0.015272	-0.450340	0.388408
4	6	0	1.920220	0.967898	-0.006271
5	6	0	-1.079282	-1.473551	-0.011277
6	6	0	-2.392204	-0.611805	-0.051166
7	6	0	-1.954285	0.894312	0.005515
8	6	0	-0.464087	0.828137	-0.333529
9	6	0	0.619669	1.834585	0.066175
10	1	0	1.807250	-2.581306	-0.048141
11	1	0	3.273748	-1.499980	-0.365452
12	1	0	-0.127493	-0.247245	1.470162
13	1	0	2.449527	1.134664	-0.952599
14	1	0	2.626146	1.225763	0.792702
15	1	0	-1.160331	-2.320058	0.678491

16	1	0	-0.852599	-1.881394	-1.004034
17	1	0	-3.052861	-0.855665	0.787657
18	1	0	-2.959997	-0.820189	-0.964284
19	1	0	-2.538275	1.522374	-0.675612
20	1	0	-2.092454	1.295438	1.018408
21	1	0	-0.365667	0.638088	-1.415635
22	1	0	0.672963	2.718555	-0.577925
23	1	0	0.448401	2.185952	1.092407

TS(2,4)*H*

Zero-point correction= 0.259044 (Hartree/Particle)
Thermal correction to Energy= 0.276419
Thermal correction to Enthalpy= 0.277363
Thermal correction to Gibbs Free Energy= 0.212960
Sum of electronic and zero-point Energies= -1164.070223
Sum of electronic and thermal Energies= -1164.052849
Sum of electronic and thermal Enthalpies= -1164.051904
Sum of electronic and thermal Free Energies= -1164.116307

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-1.017642	0.024894	0.126339
2	15	0	-2.416790	1.958779	-0.320099
3	6	0	1.145978	-0.117425	1.457747
4	6	0	0.512557	1.164499	1.087539
5	6	0	2.379920	-0.535500	0.914923
6	6	0	0.136044	-1.018993	1.848607
7	6	0	3.584634	0.385614	0.850737
8	6	0	4.259335	0.229104	-0.521026
9	6	0	3.131168	0.265761	-1.551568
10	6	0	2.001436	-0.673946	-1.153487
11	6	0	0.682099	-0.418875	-1.609411
12	15	0	-2.459665	-1.781925	-0.376788
13	1	0	-2.225032	3.132748	0.453891
14	1	0	-2.252082	2.596752	-1.577398
15	1	0	-3.839467	2.033273	-0.329476
16	1	0	1.090988	1.848247	0.469418
17	1	0	-0.039132	1.676357	1.880898
18	1	0	2.634431	-1.574194	1.136042
19	1	0	0.329038	-2.090970	1.861443
20	1	0	-0.666059	-0.680893	2.504717
21	1	0	4.293670	0.169792	1.663019
22	1	0	3.268586	1.429189	0.980678
23	1	0	4.773842	-0.741764	-0.570898
24	1	0	5.017630	1.001313	-0.702944
25	1	0	2.733983	1.288035	-1.633780
26	1	0	3.498455	-0.005031	-2.552352
27	1	0	2.296269	-1.725480	-1.154805
28	1	0	0.126877	-1.263225	-2.013482
29	1	0	-2.072938	-2.704819	-1.380328
30	1	0	-2.729788	-2.741566	0.630203
31	1	0	-3.804328	-1.638458	-0.811865
32	1	0	0.524366	0.511321	-2.155613

TS(2,4)H_t

Zero-point correction= 0.258827 (Hartree/Particle)
Thermal correction to Energy= 0.276375
Thermal correction to Enthalpy= 0.277319
Thermal correction to Gibbs Free Energy= 0.211802
Sum of electronic and zero-point Energies= -1164.057209
Sum of electronic and thermal Energies= -1164.039662
Sum of electronic and thermal Enthalpies= -1164.038718
Sum of electronic and thermal Free Energies= -1164.104234

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.082669	0.083532	-0.251898
2	15	0	2.185505	1.880068	0.848596
3	6	0	-1.102972	0.108739	-1.489618
4	6	0	-0.388019	1.348373	-1.270605
5	6	0	-2.293000	-0.244096	-0.807071
6	6	0	-0.108667	-0.902632	-1.763527
7	6	0	-3.544962	0.608323	-0.710523
8	6	0	-4.330350	0.080529	0.525333
9	6	0	-3.316188	-0.655687	1.437301
10	6	0	-1.901049	-0.188052	1.082306
11	6	0	-0.719342	-0.828720	1.536865
12	15	0	2.504382	-1.804258	0.193247
13	1	0	2.152417	3.159153	0.241391
14	1	0	1.687162	2.289538	2.110384
15	1	0	3.558595	1.915919	1.209576
16	1	0	-0.877681	2.151757	-0.721486
17	1	0	0.277926	1.700955	-2.061586
18	1	0	-2.545922	-1.298521	-0.956287
19	1	0	-0.380316	-1.948268	-1.628832
20	1	0	0.597803	-0.723845	-2.577922
21	1	0	-4.157318	0.554946	-1.619933
22	1	0	-3.278112	1.664784	-0.576915
23	1	0	-5.133069	-0.595300	0.207751
24	1	0	-4.815645	0.906522	1.058200
25	1	0	-3.515960	-0.458905	2.498784
26	1	0	-3.383801	-1.743849	1.307791
27	1	0	-1.831834	0.902680	1.181668
28	1	0	-0.050379	-0.264802	2.184159
29	1	0	-0.753350	-1.898326	1.753119
30	1	0	2.498372	-2.263764	1.531273
31	1	0	2.121044	-3.026284	-0.406951
32	1	0	3.906257	-1.964688	-0.017268

TS(2,4)*H´*

Zero-point correction= 0.232248 (Hartree/Particle)
Thermal correction to Energy= 0.245864
Thermal correction to Enthalpy= 0.246808
Thermal correction to Gibbs Free Energy= 0.191522
Sum of electronic and zero-point Energies= -820.952982
Sum of electronic and thermal Energies= -820.939367
Sum of electronic and thermal Enthalpies= -820.938423
Sum of electronic and thermal Free Energies= -820.993709

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

1	46	0	-1.083037	0.266209	0.275536
2	15	0	-2.490567	-1.258266	-0.788576
3	6	0	0.723431	1.639026	-0.285204
4	6	0	-0.218254	1.520643	-1.348925
5	6	0	1.993563	1.022369	-0.215454
6	6	0	0.013503	2.005579	0.943613
7	6	0	1.610705	-0.775752	1.224785
8	6	0	0.314359	-0.931585	1.754872
9	6	0	2.649627	0.217712	-1.302846
10	6	0	3.250662	-1.058048	-0.677289
11	6	0	2.190973	-1.729843	0.206686
12	1	0	-2.521415	-2.631662	-0.432662
13	1	0	-3.881352	-1.026144	-0.652474
14	1	0	-2.502017	-1.466981	-2.193046
15	1	0	0.036187	1.021142	-2.280755
16	1	0	-0.998347	2.275180	-1.428911
17	1	0	2.665514	1.445787	0.528162
18	1	0	0.560265	1.951238	1.881895
19	1	0	-0.694805	2.834034	0.891622
20	1	0	2.343098	-0.294362	1.869925
21	1	0	0.118449	-0.554811	2.754938
22	1	0	3.439510	0.777318	-1.827630
23	1	0	1.914745	-0.072968	-2.064745
24	1	0	3.625828	-1.746993	-1.445129
25	1	0	4.113685	-0.781182	-0.054336
26	1	0	2.638464	-2.591796	0.726349
27	1	0	1.379398	-2.129884	-0.417363
28	1	0	-0.230423	-1.840158	1.496701

TS(2,4)H_t'

Zero-point correction= 0.231875 (Hartree/Particle)
Thermal correction to Energy= 0.245817
Thermal correction to Enthalpy= 0.246762
Thermal correction to Gibbs Free Energy= 0.190717
Sum of electronic and zero-point Energies= -820.936687
Sum of electronic and thermal Energies= -820.922745
Sum of electronic and thermal Enthalpies= -820.921801
Sum of electronic and thermal Free Energies= -820.977846

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	1.206026	0.203316	-0.351389
2	15	0	2.735825	-1.072872	0.893663
3	6	0	-0.704634	1.581649	0.084170
4	6	0	0.262696	1.584954	1.133003
5	6	0	-1.953569	0.941224	0.079670
6	6	0	0.010721	1.745472	-1.192432
7	6	0	-1.449084	-1.173661	-0.356997
8	6	0	-0.505447	-1.336942	-1.376458
9	6	0	-2.833779	0.519842	1.222384
10	6	0	-3.670444	-0.703181	0.731838
11	6	0	-2.947900	-1.387535	-0.457816
12	1	0	2.810859	-2.487439	0.807261
13	1	0	4.108821	-0.826252	0.646650
14	1	0	2.814230	-1.004605	2.308552
15	1	0	0.032011	1.163532	2.110355

16	1	0	1.023621	2.362788	1.136810
17	1	0	-2.502033	1.099095	-0.849075
18	1	0	-0.540739	1.535026	-2.105805
19	1	0	0.699812	2.588196	-1.277132
20	1	0	-1.072888	-1.407241	0.643229
21	1	0	-0.804395	-1.241056	-2.418766
22	1	0	0.369085	-1.964984	-1.205888
23	1	0	-3.507523	1.321493	1.558849
24	1	0	-2.230028	0.243615	2.097042
25	1	0	-3.816100	-1.414577	1.553519
26	1	0	-4.672648	-0.383006	0.424211
27	1	0	-3.315543	-1.008231	-1.419171
28	1	0	-3.162479	-2.466766	-0.455851

Intermediates using $P(OMe)_3$ instead of PH_3

$Pd(POMe_3)_3$

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Zero-point correction=                           0.261839 (Hartree/Particle)
 Thermal correction to Energy=                    0.285600
 Thermal correction to Enthalpy=                  0.286544
 Thermal correction to Gibbs Free Energy=         0.204293
 Sum of electronic and zero-point Energies=           -1500.108972
 Sum of electronic and thermal Energies=              -1500.085211
 Sum of electronic and thermal Enthalpies=            -1500.084267
 Sum of electronic and thermal Free Energies=         -1500.166518

---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
 ---------------------------------------------------------------------
    1         46             0       -0.706504   -0.903662   -0.062619
    2         15             0        1.400208   -1.810195    0.051454
    3         15             0       -2.698633    0.228757   -0.214624
    4          8             0        1.833558   -2.869988   -1.140258
    5          8             0        2.708230   -0.825504   -0.053859
    6          8             0        1.783002   -2.584234    1.430103
    7          8             0       -3.607996    0.346838    1.160186
    8          8             0       -2.691615    1.822844   -0.602370
    9          8             0       -3.748054   -0.295931   -1.341442
   10          6             0        3.095666   -3.132790    1.650209
   11          6             0        0.832191   -3.729452   -1.698621
   12          6             0        2.779183    0.096372   -1.145834
   13          6             0       -1.842376    2.700425    0.143262
   14          6             0       -3.599349   -0.743351    2.090105
   15          6             0       -4.999418    0.374541   -1.580254
   16          1             0        3.818523   -2.329661    1.815485
   17          1             0        3.410671   -3.741240    0.797234
   18          1             0        3.021414   -3.756859    2.542989
   19          1             0       -0.123456   -3.201824   -1.811092
   20          1             0        0.684920   -4.613243   -1.066984
   21          1             0        1.194495   -4.043937   -2.680224
   22          1             0        1.839030    0.652764   -1.251130
   23          1             0        2.998132   -0.429626   -2.081415
   24          1             0        3.590616    0.791211   -0.918507
   25          1             0       -0.826127    2.292785    0.218254
   26          1             0       -2.244464    2.864256    1.148944
   27          1             0       -1.815998    3.648202   -0.398884
   28          1             0       -3.914909   -0.340280    3.055322
   29          1             0       -2.594999   -1.175759    2.182695
   30          1             0       -4.301761   -1.524607    1.777043
   31          1             0       -4.826902    1.329926   -2.082583
   32          1             0       -5.534839    0.544195   -0.641354
   33          1             0       -5.582758   -0.285580   -2.225219
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$POMe_3$

```
Zero-point correction=                           0.129342 (Hartree/Particle)
 Thermal correction to Energy=                    0.139516
 Thermal correction to Enthalpy=                  0.140460
 Thermal correction to Gibbs Free Energy=         0.093236
 Sum of electronic and zero-point Energies=           -686.642433
 Sum of electronic and thermal Energies=              -686.632259
 Sum of electronic and thermal Enthalpies=            -686.631315
 Sum of electronic and thermal Free Energies=         -686.678540

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.908737	2.033489	0.655875
2	8	0	-0.801061	1.322129	-0.589608
3	6	0	2.441861	-0.549629	0.280966
4	8	0	1.405574	0.412248	0.091594
5	6	0	-1.635872	-1.906422	0.174445
6	8	0	-0.565129	-1.021245	0.502839
7	15	0	0.047943	-0.068300	-0.726586
8	1	0	-1.715716	2.759216	0.532034
9	1	0	0.027487	2.552973	0.876870
10	1	0	-1.148088	1.349465	1.475677
11	1	0	3.323674	-0.006735	0.629994
12	1	0	2.692560	-1.065591	-0.656606
13	1	0	2.152007	-1.293596	1.031396
14	1	0	-1.639495	-2.707174	0.918867
15	1	0	-1.509561	-2.348524	-0.823237
16	1	0	-2.600594	-1.385221	0.207477

TS (1Z, 2Z) – $P(OMe)_3$

Zero-point correction= 0.509223 (Hartree/Particle)
Thermal correction to Energy= 0.549047
Thermal correction to Enthalpy= 0.549991
Thermal correction to Gibbs Free Energy= 0.426117
Sum of electronic and zero-point Energies= -2078.998608
Sum of electronic and thermal Energies= -2078.958784
Sum of electronic and thermal Enthalpies= -2078.957840
Sum of electronic and thermal Free Energies= -2079.081714

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	3.805239	-1.185145	0.246318
2	8	0	4.809861	-0.783324	1.505598
3	8	0	3.984100	-2.825358	0.406888
4	8	0	4.748264	-0.999777	-1.081169
5	6	0	6.040171	-1.622622	-1.186139
6	6	0	4.794806	0.546452	2.035020
7	6	0	3.588001	-3.446668	1.629587
8	46	0	1.703522	-0.194835	-0.066049
9	1	0	5.933354	-2.701558	-1.324533
10	1	0	6.640800	-1.427094	-0.292413
11	1	0	6.525248	-1.181842	-2.060101
12	1	0	3.787797	0.976251	2.024753
13	1	0	5.466663	1.195104	1.459342
14	1	0	5.157722	0.483936	3.064484
15	1	0	2.602679	-3.095267	1.962532
16	1	0	4.320008	-3.249086	2.419345
17	1	0	3.534700	-4.521291	1.437697
18	15	0	1.650138	2.146702	-0.132111
19	8	0	2.547921	3.000716	-1.238129
20	8	0	0.249046	3.005281	-0.345655
21	8	0	2.077757	2.804592	1.307474
22	6	0	-0.368002	3.020964	-1.633439
23	6	0	3.787289	2.460931	-1.708891
24	6	0	2.026749	4.223202	1.537577

25	1	0	-0.451831	2.011001	-2.054307
26	1	0	0.199030	3.650135	-2.327156
27	1	0	-1.371300	3.432658	-1.499172
28	1	0	4.022867	2.978334	-2.642642
29	1	0	3.716359	1.383441	-1.890953
30	1	0	4.590392	2.646785	-0.985186
31	1	0	0.989794	4.564057	1.591257
32	1	0	2.548928	4.764743	0.742696
33	1	0	2.526229	4.398730	2.493150
34	6	0	-2.087281	-2.767128	-0.611964
35	6	0	-3.379625	-2.267057	-1.200967
36	6	0	-4.557873	-2.344630	-0.211074
37	6	0	-5.882027	-1.851525	-0.831910
38	6	0	-7.031708	-2.000908	0.120245
39	6	0	-7.829279	-1.050437	0.637175
40	6	0	-0.997490	-2.024720	-0.439308
41	6	0	0.368746	-2.141629	0.063211
42	6	0	-0.527725	-0.660979	-0.678051
43	6	0	-7.748213	0.398863	0.348980
44	8	0	-6.966240	0.972540	-0.388007
45	8	0	-8.708385	1.058526	1.048283
46	6	0	-8.735776	2.478672	0.858425
47	1	0	-2.063442	-3.812084	-0.295393
48	1	0	-3.633713	-2.860216	-2.093659
49	1	0	-3.255065	-1.230639	-1.539150
50	1	0	-4.325621	-1.742001	0.675967
51	1	0	-4.673808	-3.380733	0.139280
52	1	0	-5.787979	-0.813234	-1.153822
53	1	0	-6.094897	-2.461057	-1.724511
54	1	0	-7.227596	-3.024141	0.447288
55	1	0	-8.616136	-1.330339	1.331424
56	1	0	0.493799	-2.187020	1.145149
57	1	0	1.071362	-2.747995	-0.505843
58	1	0	-0.935982	0.135131	-0.057734
59	1	0	-0.329716	-0.382203	-1.713072
60	1	0	-8.919146	2.725162	-0.191351
61	1	0	-7.786480	2.928047	1.163724
62	1	0	-9.550821	2.843118	1.484947

TS (2Z, 3Z) – $P(OMe)_3$

Zero-point correction= 0.510891 (Hartree/Particle)
Thermal correction to Energy= 0.549684
Thermal correction to Enthalpy= 0.550628
Thermal correction to Gibbs Free Energy= 0.433211
Sum of electronic and zero-point Energies= -2079.001004
Sum of electronic and thermal Energies= -2078.962211
Sum of electronic and thermal Enthalpies= -2078.961267
Sum of electronic and thermal Free Energies= -2079.078684

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.252810	-1.806607	-1.855044
2	6	0	0.540127	-0.983791	-2.983009
3	6	0	1.373430	-2.572650	-1.348409

4	6	0	-0.810043	-1.638290	-0.918389
5	46	0	1.529992	-0.562203	-0.603865
6	6	0	-2.051201	-0.845001	-1.206661
7	6	0	-2.845442	-0.478031	0.055274
8	6	0	-4.145635	0.288393	-0.262988
9	6	0	-4.871870	0.703742	0.981659
10	6	0	-6.141484	0.454545	1.347665
11	6	0	-7.138118	-0.300074	0.557450
12	8	0	-6.995750	-0.809138	-0.539721
13	8	0	-8.312304	-0.363619	1.241899
14	6	0	-9.366531	-1.070511	0.578106
15	15	0	3.383349	-0.788264	0.694768
16	8	0	3.125353	-1.286091	2.243376
17	8	0	4.623772	-1.804712	0.357207
18	8	0	4.248870	0.583797	0.866156
19	6	0	5.409782	0.635354	1.716917
20	6	0	1.913426	-0.915359	2.921972
21	6	0	4.465752	-3.224552	0.433850
22	1	0	-0.229700	-0.357046	-3.420032
23	1	0	1.378159	-1.241898	-3.620585
24	1	0	2.192047	-2.810144	-2.024195
25	1	0	1.191015	-3.300318	-0.560665
26	1	0	-0.888843	-2.398364	-0.143434
27	1	0	-2.718380	-1.406219	-1.889383
28	1	0	-1.797356	0.078068	-1.743630
29	1	0	-2.205688	0.125691	0.712339
30	1	0	-3.094231	-1.393014	0.610815
31	1	0	-3.876508	1.202981	-0.816425
32	1	0	-4.799333	-0.302639	-0.906553
33	1	0	-4.271314	1.278222	1.690154
34	1	0	-6.507484	0.825473	2.300658
35	1	0	-9.081770	-2.111073	0.397221
36	1	0	-9.603853	-0.601089	-0.380980
37	1	0	-10.223657	-1.020339	1.251027
38	1	0	6.234921	0.078112	1.266029
39	1	0	5.183976	0.224684	2.705040
40	1	0	5.675812	1.690455	1.806584
41	1	0	1.036448	-1.145554	2.307554
42	1	0	1.909939	0.153806	3.154749
43	1	0	1.889950	-1.498618	3.845293
44	1	0	3.712071	-3.577143	-0.277515
45	1	0	4.187498	-3.529978	1.447135
46	1	0	5.434398	-3.656365	0.172933
47	15	0	1.012940	1.696343	-0.243103
48	8	0	1.965609	2.831905	-0.950354
49	8	0	-0.447371	2.312338	-0.667385
50	8	0	1.008373	2.112720	1.331404
51	6	0	-0.701724	2.683957	-2.029840
52	6	0	3.203745	2.493187	-1.596839
53	6	0	0.743403	3.464590	1.750408
54	1	0	-0.357208	1.908655	-2.722062
55	1	0	-0.205603	3.630403	-2.264375
56	1	0	-1.783998	2.798149	-2.122026
57	1	0	3.384994	3.270124	-2.343842
58	1	0	3.133641	1.515579	-2.085315
59	1	0	4.017249	2.471824	-0.868294
60	1	0	-0.282503	3.747544	1.500960
61	1	0	1.444676	4.158002	1.276989
62	1	0	0.881663	3.481195	2.833243

TS (3Z´, 4a´) – $P(OMe)_3$

Zero-point correction= 0.381874 (Hartree/Particle)
Thermal correction to Energy= 0.407581
Thermal correction to Enthalpy= 0.408526
Thermal correction to Gibbs Free Energy= 0.324950
Sum of electronic and zero-point Energies= -1392.333408
Sum of electronic and thermal Energies= -1392.307701
Sum of electronic and thermal Enthalpies= -1392.306757
Sum of electronic and thermal Free Energies= -1392.390332

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.418919	-0.492752	0.113359
2	6	0	-2.278646	-1.978988	0.407444
3	6	0	-1.230727	-2.315892	-0.576832
4	6	0	-2.922139	-0.609656	0.237684
5	6	0	-2.550318	-2.721564	1.510364
6	6	0	-2.183980	1.208056	0.570626
7	6	0	-0.758188	1.467795	0.922909
8	6	0	-3.642951	-0.336404	-1.078175
9	6	0	0.050154	2.478547	0.228764
10	8	0	-0.111559	2.966277	-0.877962
11	8	0	1.114380	2.857656	1.020395
12	6	0	2.002324	3.801599	0.415503
13	6	0	-4.062905	1.135455	-1.063990
14	6	0	-2.813532	1.907397	-0.631885
15	1	0	-1.466063	-2.152225	-1.629987
16	1	0	-0.734913	-3.272066	-0.415701
17	1	0	-3.617907	-0.491167	1.068702
18	1	0	-3.246627	-2.381706	2.272386
19	1	0	-2.085219	-3.691599	1.663692
20	1	0	-2.794908	1.302863	1.468909
21	1	0	-0.548384	1.434922	1.990320
22	1	0	-4.505094	-1.011104	-1.171065
23	1	0	-2.985256	-0.532645	-1.933540
24	1	0	1.474099	4.722113	0.150839
25	1	0	2.455018	3.385641	-0.489304
26	1	0	2.768691	4.007804	1.165489
27	1	0	-4.433190	1.473166	-2.038328
28	1	0	-4.877419	1.280315	-0.339382
29	1	0	-3.043585	2.946972	-0.364369
30	1	0	-2.091929	1.953677	-1.448928
31	15	0	1.761138	-0.732901	-0.275446
32	8	0	2.753355	-0.786604	1.025081
33	8	0	2.355659	-2.031310	-1.062612
34	8	0	2.338478	0.437778	-1.228619
35	6	0	2.376324	-3.316300	-0.428637
36	6	0	2.413482	-0.092616	2.241187
37	6	0	3.710972	0.449435	-1.670114
38	1	0	1.400124	-3.558391	0.003614
39	1	0	3.140929	-3.342243	0.353297
40	1	0	2.616107	-4.041450	-1.208690
41	1	0	3.282579	-0.191359	2.895089
42	1	0	1.543431	-0.558401	2.715271
43	1	0	2.202556	0.961586	2.047117
44	1	0	3.889729	-0.369761	-2.370314
45	1	0	4.391503	0.365331	-0.817594

46	1	0	3.857211	1.408267	-2.169701

TS (2Z,6) – $P(OMe)_3$ calculado con G03 en vacío

Zero-point correction= 0.511862 (Hartree/Particle)
Thermal correction to Energy= 0.549758
Thermal correction to Enthalpy= 0.550702
Thermal correction to Gibbs Free Energy= 0.438684
Sum of electronic and zero-point Energies= -2078.995559
Sum of electronic and thermal Energies= -2078.957663
Sum of electronic and thermal Enthalpies= -2078.956719
Sum of electronic and thermal Free Energies= -2079.068738

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.104499	-1.227051	-0.281881
2	8	0	3.140945	-1.009270	0.975507
3	8	0	2.086181	-2.852170	-0.244275
4	8	0	3.029875	-0.995000	-1.606231
5	6	0	4.231375	-1.760321	-1.826092
6	6	0	3.664687	0.287501	1.293860
7	6	0	1.405346	-3.547913	0.819415
8	46	0	0.040476	-0.117610	-0.759282
9	6	0	-1.969151	-1.166700	-1.720008
10	6	0	-1.740399	0.248707	-1.937546
11	6	0	-3.118265	-1.728013	-1.084025
12	6	0	-0.706020	-1.850368	-1.848538
13	6	0	-4.471659	-1.042904	-1.323166
14	6	0	-5.101022	-0.592321	0.019999
15	6	0	-3.943796	-0.399818	0.999435
16	6	0	-3.066754	-1.639343	0.883030
17	6	0	-1.837658	-1.787693	1.580154
18	6	0	-1.052494	-0.734939	2.112133
19	8	0	-1.208555	0.495061	2.018418
20	8	0	0.014697	-1.236912	2.864130
21	6	0	0.721188	-0.270260	3.630866
22	1	0	3.977862	-2.779854	-2.126647
23	1	0	4.848866	-1.789284	-0.923452
24	1	0	4.772235	-1.257271	-2.630144
25	1	0	2.871623	1.035902	1.358822
26	1	0	4.405316	0.593570	0.544823
27	1	0	4.156507	0.190681	2.264245
28	1	0	0.362900	-3.226073	0.880462
29	1	0	1.901355	-3.362704	1.775275
30	1	0	1.461831	-4.608781	0.567132
31	1	0	-2.495557	0.956367	-1.608417
32	1	0	-1.233779	0.538206	-2.860792
33	1	0	-3.135465	-2.812788	-1.183703
34	1	0	-0.609846	-2.857369	-1.448254
35	1	0	-0.115797	-1.670222	-2.748674
36	1	0	-5.149900	-1.713277	-1.865885
37	1	0	-4.333371	-0.168647	-1.970199
38	1	0	-5.771387	-1.374164	0.403537
39	1	0	-5.710508	0.311125	-0.103026
40	1	0	-3.359705	0.499016	0.782729
41	1	0	-4.298601	-0.296200	2.033518
42	1	0	-3.675658	-2.543906	0.968888

43	1	0	-1.526296	-2.792844	1.847961
44	1	0	0.092541	0.134206	4.434704
45	1	0	1.064087	0.562770	3.012752
46	1	0	1.573769	-0.798267	4.067050
47	15	0	0.224621	2.143535	-0.080969
48	8	0	0.857221	3.130588	-1.249036
49	8	0	-1.088562	3.037078	0.258389
50	8	0	1.138408	2.456116	1.230035
51	6	0	-1.837099	3.755124	-0.728449
52	6	0	1.958742	2.669660	-2.038799
53	6	0	1.103160	3.733112	1.894708
54	1	0	-2.076993	3.128616	-1.592449
55	1	0	-1.283485	4.634866	-1.068085
56	1	0	-2.763358	4.062691	-0.238877
57	1	0	1.989761	3.292847	-2.935674
58	1	0	1.833589	1.618827	-2.325998
59	1	0	2.900764	2.781846	-1.489140
60	1	0	0.160493	3.844224	2.433625
61	1	0	1.225667	4.551929	1.178936
62	1	0	1.939079	3.731780	2.597286

TS (2Z,6) – $P(OMe)_3$ calculado con G09 y PCM

Zero-point correction= 0.511662 (Hartree/Particle)
Thermal correction to Energy= 0.549211
Thermal correction to Enthalpy= 0.550155
Thermal correction to Gibbs Free Energy= 0.439874
Sum of electronic and zero-point Energies= -2079.024465
Sum of electronic and thermal Energies= -2078.986916
Sum of electronic and thermal Enthalpies= -2078.985972
Sum of electronic and thermal Free Energies= -2079.096253

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.821918	-1.731921	0.325710
2	8	0	2.205890	-1.672168	1.911912
3	8	0	1.598165	-3.348198	0.215714
4	8	0	3.226529	-1.609294	-0.478609
5	6	0	4.367604	-2.439428	-0.153303
6	6	0	2.158811	-0.438509	2.663534
7	6	0	0.610265	-3.996342	1.036706
8	46	0	0.192239	-0.328849	-0.675966
9	6	0	-1.930561	-1.045663	-1.792952
10	6	0	-1.391241	0.278606	-2.046016
11	6	0	-3.214965	-1.342695	-1.286821
12	6	0	-0.821954	-1.963430	-1.685843
13	6	0	-4.446017	-0.531152	-1.636960
14	6	0	-5.437903	-0.695524	-0.478868
15	6	0	-4.653674	-0.375622	0.795852
16	6	0	-3.294224	-1.070939	0.794025
17	6	0	-2.171829	-0.522289	1.461770
18	6	0	-2.011933	0.840443	1.849277
19	8	0	-2.697002	1.835672	1.559983
20	8	0	-0.937044	0.992706	2.724009
21	6	0	-0.750708	2.303738	3.257996

22	1	0	4.175426	-3.474143	-0.444995
23	1	0	4.586458	-2.386790	0.916083
24	1	0	5.205893	-2.038417	-0.723880
25	1	0	1.179436	0.035444	2.563958
26	1	0	2.942749	0.244089	2.328723
27	1	0	2.330923	-0.719022	3.704302
28	1	0	-0.361985	-3.499239	0.950917
29	1	0	0.928421	-4.001836	2.082374
30	1	0	0.526461	-5.019874	0.668165
31	1	0	-2.013414	1.147217	-1.845832
32	1	0	-0.755402	0.392130	-2.925944
33	1	0	-3.412237	-2.415719	-1.258711
34	1	0	-0.990036	-2.937756	-1.231821
35	1	0	-0.090362	-1.975870	-2.497382
36	1	0	-4.892852	-0.856423	-2.588629
37	1	0	-4.191349	0.530429	-1.752698
38	1	0	-5.798800	-1.734208	-0.454824
39	1	0	-6.319377	-0.051538	-0.588008
40	1	0	-4.499303	0.701824	0.879727
41	1	0	-5.208861	-0.696126	1.689820
42	1	0	-3.370802	-2.149593	0.932345
43	1	0	-1.411722	-1.203725	1.831087
44	1	0	-1.656156	2.660801	3.758785
45	1	0	-0.470493	3.018008	2.478666
46	1	0	0.061214	2.214388	3.983545
47	15	0	1.191005	1.818508	-0.546294
48	8	0	1.625089	2.381314	-2.028352
49	8	0	0.429078	3.158114	-0.023086
50	8	0	2.544505	1.913809	0.345824
51	6	0	-0.840173	3.573413	-0.574448
52	6	0	2.335930	1.528946	-2.945154
53	6	0	3.306968	3.139504	0.458197
54	1	0	-1.642239	2.962798	-0.153114
55	1	0	-0.826019	3.520056	-1.666443
56	1	0	-0.972412	4.613132	-0.268739
57	1	0	2.385197	2.068237	-3.892400
58	1	0	1.810415	0.579742	-3.092149
59	1	0	3.349987	1.333120	-2.582699
60	1	0	2.778755	3.850822	1.096685
61	1	0	3.478475	3.578998	-0.527452
62	1	0	4.259122	2.863298	0.912628

TS (7Z,5a) – $P(OMe)_3$

Zero-point correction= 0.513216 (Hartree/Particle)
Thermal correction to Energy= 0.550796
Thermal correction to Enthalpy= 0.551740
Thermal correction to Gibbs Free Energy= 0.439073
Sum of electronic and zero-point Energies= -2079.015205
Sum of electronic and thermal Energies= -2078.977625
Sum of electronic and thermal Enthalpies= -2078.976681
Sum of electronic and thermal Free Energies= -2079.089348

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.127646	-1.458907	-0.041146

2	15	0	1.027186	2.040647	-0.207374
3	8	0	3.119032	-1.482674	1.274201
4	8	0	2.238854	-3.051132	-0.434618
5	8	0	3.058333	-0.848199	-1.235287
6	8	0	1.218819	2.513714	-1.781531
7	8	0	0.311164	3.418224	0.334232
8	8	0	2.502230	2.283263	0.465069
9	6	0	4.378605	-1.359007	-1.496894
10	6	0	2.956910	-0.516663	2.326605
11	6	0	2.230489	-4.087286	0.553457
12	6	0	-0.926654	3.863528	-0.247506
13	6	0	1.391425	1.536312	-2.815960
14	6	0	3.202059	3.533842	0.328238
15	46	0	0.120667	-0.360762	0.131708
16	6	0	-2.330147	-2.182242	0.145163
17	6	0	-0.921521	-2.321197	-0.042443
18	6	0	-3.282722	-1.703263	-0.927677
19	6	0	-2.910197	-2.308309	1.390460
20	6	0	-2.704914	-1.167383	-2.252450
21	6	0	-3.756402	-0.153046	-2.733144
22	6	0	-4.148336	0.583811	-1.442418
23	6	0	-4.206228	-0.519628	-0.348109
24	6	0	-3.856396	-0.104782	1.059798
25	6	0	-2.681889	0.570833	1.376230
26	8	0	-1.744062	0.830318	0.554897
27	8	0	-2.563064	0.942124	2.697318
28	6	0	-1.338652	1.548916	3.086059
29	1	0	4.326704	-2.401786	-1.820465
30	1	0	5.005610	-1.277841	-0.604017
31	1	0	4.793373	-0.741248	-2.295737
32	1	0	1.914826	-0.481438	2.663670
33	1	0	3.257535	0.479006	1.991766
34	1	0	3.596174	-0.849915	3.147343
35	1	0	1.443333	-3.935078	1.299783
36	1	0	3.197222	-4.140389	1.062336
37	1	0	2.038902	-5.020413	0.019175
38	1	0	-1.680753	3.074986	-0.190349
39	1	0	-0.769656	4.167376	-1.286860
40	1	0	-1.247216	4.726281	0.341064
41	1	0	1.051767	1.997791	-3.746668
42	1	0	0.802028	0.634396	-2.615986
43	1	0	2.444266	1.252857	-2.903953
44	1	0	2.696038	4.317315	0.897799
45	1	0	3.264471	3.826858	-0.723920
46	1	0	4.206073	3.371205	0.726152
47	1	0	-0.579402	-2.545548	-1.053028
48	1	0	-0.430860	-2.941676	0.704412
49	1	0	-3.959023	-2.534622	-1.172883
50	1	0	-2.308179	-2.491249	2.278832
51	1	0	-3.972265	-2.494461	1.500910
52	1	0	-2.510048	-1.961806	-2.983088
53	1	0	-1.757741	-0.646032	-2.065029
54	1	0	-4.623716	-0.682166	-3.153562
55	1	0	-3.378380	0.519539	-3.512574
56	1	0	-3.368089	1.305184	-1.187047
57	1	0	-5.096108	1.127843	-1.527309
58	1	0	-5.232893	-0.903909	-0.316059
59	1	0	-4.626488	-0.125231	1.823777
60	1	0	-1.060792	2.378877	2.430155
61	1	0	-0.515220	0.821349	3.085068
62	1	0	-1.497670	1.911160	4.104840

TS (7E,5b) – $P(OMe)_3$

Zero-point correction= 0.513386 (Hartree/Particle)
Thermal correction to Energy= 0.550809
Thermal correction to Enthalpy= 0.551754
Thermal correction to Gibbs Free Energy= 0.440361
Sum of electronic and zero-point Energies= -2079.018954
Sum of electronic and thermal Energies= -2078.981531
Sum of electronic and thermal Enthalpies= -2078.980586
Sum of electronic and thermal Free Energies= -2079.091979

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.974181	-1.743088	0.014114
2	8	0	3.013876	-1.806411	1.289407
3	8	0	1.768983	-3.362265	-0.185518
4	8	0	2.932882	-1.465674	-1.276671
5	6	0	4.119868	-2.245664	-1.514331
6	6	0	3.075671	-0.734321	2.244204
7	6	0	1.536533	-4.229222	0.929834
8	15	0	1.542102	1.878859	-0.413048
9	8	0	1.670119	2.214925	-2.028611
10	8	0	1.146461	3.391049	0.094133
11	8	0	3.095715	1.868715	0.108123
12	6	0	-0.026765	4.041084	-0.428529
13	6	0	1.472691	1.167524	-2.989737
14	6	0	4.003239	2.944973	-0.192854
15	46	0	0.221523	-0.263645	0.107994
16	6	0	-2.547863	-1.592111	0.093807
17	6	0	-1.185582	-1.983153	-0.091696
18	6	0	-3.324863	-0.892682	-0.994869
19	6	0	-3.159634	-1.625904	1.326583
20	6	0	-4.551697	-1.664376	-1.547898
21	6	0	-5.572793	-0.575112	-1.909113
22	6	0	-5.449987	0.410025	-0.737078
23	6	0	-3.933962	0.488126	-0.436655
24	6	0	-3.603674	0.759242	1.004902
25	6	0	-2.323402	1.175346	1.344478
26	8	0	-1.365345	1.266010	0.508250
27	8	0	-2.115447	1.476501	2.670235
28	6	0	-0.799098	1.868204	3.034697
29	1	0	3.858117	-3.289619	-1.704475
30	1	0	4.797602	-2.182604	-0.657955
31	1	0	4.597845	-1.814089	-2.395720
32	1	0	2.069787	-0.443501	2.567258
33	1	0	3.579327	0.136052	1.817526
34	1	0	3.638008	-1.117696	3.098743
35	1	0	0.789580	-3.818088	1.618637
36	1	0	2.466347	-4.405255	1.478194
37	1	0	1.162143	-5.169106	0.518351
38	1	0	-0.412643	2.663681	2.390415
39	1	0	-0.902688	3.396614	-0.321105
40	1	0	0.125432	4.306749	-1.479074
41	1	0	-0.159830	4.950020	0.162797
42	1	0	1.387283	1.654131	-3.964375
43	1	0	0.554393	0.606823	-2.779665
44	1	0	2.317200	0.472595	-2.992549
45	1	0	3.710031	3.851307	0.342896

46	1	0	4.020840	3.142908	-1.268518
47	1	0	4.991072	2.617525	0.138442
48	1	0	-0.891745	-2.216586	-1.117472
49	1	0	-0.821323	-2.721870	0.617637
50	1	0	-2.650438	-0.666460	-1.828411
51	1	0	-2.622216	-1.941281	2.218669
52	1	0	-4.237417	-1.574007	1.426271
53	1	0	-4.967774	-2.310115	-0.763445
54	1	0	-4.288752	-2.312538	-2.391886
55	1	0	-6.589051	-0.963370	-2.044571
56	1	0	-5.282604	-0.082785	-2.847962
57	1	0	-5.884196	1.393944	-0.948525
58	1	0	-5.984594	0.005717	0.134505
59	1	0	-3.489407	1.280977	-1.050687
60	1	0	-4.393745	0.866506	1.740837
61	1	0	-0.102033	1.020358	2.985088
62	1	0	-0.868888	2.219482	4.067155

TS (4a,5a) – $P(OMe)_3$

Zero-point correction= 0.514074 (Hartree/Particle)
Thermal correction to Energy= 0.551619
Thermal correction to Enthalpy= 0.552564
Thermal correction to Gibbs Free Energy= 0.440612
Sum of electronic and zero-point Energies= -2079.009255
Sum of electronic and thermal Energies= -2078.971709
Sum of electronic and thermal Enthalpies= -2078.970765
Sum of electronic and thermal Free Energies= -2079.082717

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.305194	-0.089588	-0.208963
2	15	0	2.549348	-0.987778	-0.230378
3	15	0	-0.175251	2.182876	-0.356040
4	8	0	3.694492	-0.492994	0.858379
5	8	0	2.827978	-2.609005	-0.097160
6	8	0	3.268758	-0.767647	-1.687937
7	8	0	0.546440	3.053885	-1.570950
8	8	0	-1.685445	2.808702	-0.601495
9	8	0	0.193798	3.030473	0.999135
10	6	0	4.569139	-1.308975	-1.980592
11	6	0	3.557881	0.771123	1.516159
12	6	0	2.656461	-3.238520	1.182461
13	6	0	-2.368458	2.474306	-1.811419
14	6	0	1.875838	2.741145	-1.995987
15	6	0	-0.067709	4.441770	1.099681
16	1	0	4.519686	-2.397789	-2.061256
17	1	0	5.287828	-1.031871	-1.203141
18	1	0	4.875089	-0.877552	-2.936325
19	1	0	2.507622	1.005231	1.717933
20	1	0	3.998091	1.570623	0.907728
21	1	0	4.102709	0.697888	2.460781
22	1	0	1.813199	-2.809451	1.734118
23	1	0	3.566896	-3.125034	1.779850
24	1	0	2.476213	-4.299399	0.989340
25	1	0	-2.345984	1.391890	-1.995100
26	1	0	-1.921391	2.997721	-2.663317
27	1	0	-3.405796	2.794728	-1.687837

28	1	0	2.020262	3.232562	-2.961760
29	1	0	2.021917	1.661596	-2.107739
30	1	0	2.613860	3.131031	-1.283915
31	1	0	-1.137774	4.622136	1.231292
32	1	0	0.283439	4.967676	0.206995
33	1	0	0.480611	4.795906	1.975823
34	6	0	-2.195085	-1.942201	-1.553215
35	6	0	-2.591839	-1.535410	-2.769156
36	6	0	-3.111638	-2.454963	-0.460995
37	6	0	-0.769185	-1.891491	-1.154708
38	6	0	-4.609952	-2.170455	-0.624664
39	6	0	-4.768473	-0.678271	-0.240433
40	6	0	-3.541229	-0.329448	0.652169
41	6	0	-2.732706	-1.644732	0.805069
42	6	0	-1.218428	-1.583077	0.951207
43	6	0	-0.635397	-0.777822	2.079827
44	8	0	0.404009	-1.073084	2.662748
45	8	0	-1.433615	0.232531	2.504146
46	6	0	-0.925474	1.012804	3.595578
47	1	0	-3.630023	-1.573980	-3.085054
48	1	0	-1.877753	-1.166029	-3.501224
49	1	0	-2.910117	-3.526549	-0.311201
50	1	0	-0.153419	-1.410075	-1.928846
51	1	0	-0.332406	-2.856537	-0.901905
52	1	0	-5.162527	-2.804969	0.079426
53	1	0	-4.994715	-2.403726	-1.623018
54	1	0	-5.717903	-0.498533	0.275277
55	1	0	-4.774225	-0.051491	-1.138332
56	1	0	-2.920411	0.439878	0.187048
57	1	0	-3.836497	0.062534	1.627195
58	1	0	-3.117042	-2.186238	1.684309
59	1	0	-0.805888	-2.580527	1.082050
60	1	0	-0.077236	1.614442	3.260612
61	1	0	-0.620489	0.368828	4.424053
62	1	0	-1.749987	1.662107	3.893857

TS (2Z,4a) – $P(OMe)_3$

Zero-point correction= 0.512691 (Hartree/Particle)
Thermal correction to Energy= 0.550045
Thermal correction to Enthalpy= 0.550989
Thermal correction to Gibbs Free Energy= 0.440873
Sum of electronic and zero-point Energies= -2079.005309
Sum of electronic and thermal Energies= -2078.967955
Sum of electronic and thermal Enthalpies= -2078.967011
Sum of electronic and thermal Free Energies= -2079.077127

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.194383	-0.346312	-0.633723
2	6	0	-1.845451	-1.259425	-1.752328
3	6	0	-1.450557	0.115508	-1.991154
4	6	0	-3.069173	-1.668495	-1.166542
5	6	0	-0.655037	-2.063533	-1.679485
6	6	0	-4.395107	-1.005027	-1.490546
7	6	0	-5.296032	-1.193805	-0.263446
8	6	0	-4.459233	-0.733321	0.932910
9	6	0	-3.045098	-1.309252	0.845344

10	6	0	-1.907443	-0.664518	1.405996
11	6	0	-1.700028	0.696986	1.785958
12	8	0	-0.744158	1.114948	2.456577
13	8	0	-2.676179	1.603361	1.384773
14	6	0	-2.602710	2.875838	2.029937
15	15	0	1.973643	-1.549079	0.350528
16	15	0	1.055202	1.858954	-0.463497
17	8	0	2.244436	-1.576753	1.954436
18	8	0	2.013910	-3.167690	0.099383
19	8	0	3.394860	-1.152152	-0.338193
20	8	0	1.729114	2.339289	-1.892737
21	8	0	0.178223	3.206610	-0.203469
22	8	0	2.230647	2.088897	0.629561
23	6	0	4.613034	-1.842327	0.005424
24	6	0	2.046769	-0.417589	2.804838
25	6	0	1.139005	-4.025754	0.843668
26	6	0	-0.963550	3.519242	-1.014663
27	6	0	2.534585	1.418293	-2.640992
28	6	0	2.829462	3.382058	0.843500
29	1	0	-2.161153	0.904214	-1.760827
30	1	0	-0.844525	0.314278	-2.877427
31	1	0	-3.155886	-2.756085	-1.116863
32	1	0	-0.719833	-3.058286	-1.243314
33	1	0	0.070828	-1.989142	-2.492304
34	1	0	-4.853579	-1.430829	-2.395054
35	1	0	-4.256431	0.067419	-1.678932
36	1	0	-5.558061	-2.257612	-0.164039
37	1	0	-6.238499	-0.638276	-0.344964
38	1	0	-4.409816	0.355919	0.951273
39	1	0	-4.909944	-1.052359	1.883300
40	1	0	-3.034511	-2.379095	1.063023
41	1	0	-1.109398	-1.306499	1.768382
42	1	0	-1.643120	3.363943	1.843673
43	1	0	-2.735489	2.775073	3.112854
44	1	0	4.603263	-2.854220	-0.407181
45	1	0	4.739248	-1.887613	1.090883
46	1	0	5.426526	-1.264821	-0.437678
47	1	0	1.060090	0.029941	2.651043
48	1	0	2.829622	0.320665	2.612292
49	1	0	2.135423	-0.792313	3.826781
50	1	0	0.102040	-3.673974	0.795516
51	1	0	1.455034	-4.080269	1.889033
52	1	0	1.207146	-5.012806	0.381341
53	1	0	-1.807365	2.883979	-0.734655
54	1	0	-0.732144	3.407845	-2.078621
55	1	0	-1.207355	4.563571	-0.807708
56	1	0	2.796572	1.924241	-3.572941
57	1	0	1.980469	0.499271	-2.863013
58	1	0	3.445156	1.156187	-2.092907
59	1	0	2.142256	4.023740	1.399376
60	1	0	3.090410	3.853357	-0.108503
61	1	0	3.733482	3.205466	1.429572
62	1	0	-3.422188	3.465983	1.611243

Optimized stationary points containing $P(OMe)_3$ using G09 and PCM (acetonitrile)

1Z – PCM (acetonitrile)

```
Zero-point correction=                           0.248705 (Hartree/Particle)
 Thermal correction to Energy=                    0.263412
 Thermal correction to Enthalpy=                  0.264356
 Thermal correction to Gibbs Free Energy=         0.204066
 Sum of electronic and zero-point Energies=           -578.926083
 Sum of electronic and thermal Energies=              -578.911376
 Sum of electronic and thermal Enthalpies=            -578.910432
 Sum of electronic and thermal Free Energies=         -578.970722
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.401909	-0.374627	-0.221281
2	6	0	5.350087	0.364758	0.626929
3	6	0	3.157463	-0.784119	-0.427566
4	6	0	5.803816	-0.349587	-0.661006
5	6	0	1.986683	-0.463427	0.465973
6	6	0	0.896267	0.353577	-0.253779
7	6	0	-0.325308	0.625012	0.649619
8	6	0	-1.336551	1.498896	-0.030921
9	6	0	-2.628995	1.249357	-0.308466
10	6	0	-3.370277	0.014185	0.023725
11	8	0	-2.952613	-0.977544	0.602398
12	8	0	-4.648014	0.113636	-0.415563
13	6	0	-5.489126	-1.023366	-0.159635
14	1	0	5.655156	-0.065213	1.580512
15	1	0	5.328188	1.454119	0.622175
16	1	0	2.941322	-1.387645	-1.311666
17	1	0	6.081034	0.269650	-1.513729
18	1	0	6.408442	-1.250042	-0.555989
19	1	0	2.336175	0.086032	1.349070
20	1	0	1.536330	-1.399252	0.830966
21	1	0	0.568435	-0.183825	-1.153714
22	1	0	1.324484	1.305007	-0.596916
23	1	0	-0.779825	-0.314294	0.968537
24	1	0	0.023764	1.150445	1.552148
25	1	0	-0.955789	2.468698	-0.355406
26	1	0	-3.216345	2.003985	-0.823143
27	1	0	-5.088047	-1.915978	-0.646935
28	1	0	-6.462846	-0.767372	-0.577055
29	1	0	-5.571269	-1.207012	0.914911

$Pd(POMe_3)_3$ – PCM (acetonitrile)

```
Zero-point correction=                           0.260894 (Hartree/Particle)
 Thermal correction to Energy=                    0.284991
 Thermal correction to Enthalpy=                  0.285935
 Thermal correction to Gibbs Free Energy=         0.202116
```

```
 Sum of electronic and zero-point Energies=          -1500.120369
 Sum of electronic and thermal Energies=             -1500.096272
 Sum of electronic and thermal Enthalpies=           -1500.095328
 Sum of electronic and thermal Free Energies=        -1500.179147
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.000058	-0.125516	0.000070
2	15	0	-2.296274	-0.038514	-0.057223
3	15	0	2.296339	-0.038469	0.057183
4	8	0	-3.109885	-0.132528	1.371990
5	8	0	-3.041948	1.297891	-0.644512
6	8	0	-3.000617	-1.161276	-1.003769
7	8	0	3.109798	-0.132835	-1.372068
8	8	0	3.042053	1.298061	0.644088
9	8	0	3.000670	-1.161031	1.003940
10	6	0	-4.435666	-1.233956	-1.165200
11	6	0	-2.609394	-0.997417	2.406726
12	6	0	-2.647684	2.583661	-0.138655
13	6	0	2.647753	2.583734	0.137954
14	6	0	2.609397	-0.998310	-2.406371
15	6	0	4.435718	-1.233607	1.165522
16	1	0	-4.792465	-0.386809	-1.755862
17	1	0	-4.932502	-1.244153	-0.191644
18	1	0	-4.637476	-2.166946	-1.693168
19	1	0	-1.515490	-0.945494	2.466310
20	1	0	-2.915737	-2.032427	2.223158
21	1	0	-3.043831	-0.650376	3.346028
22	1	0	-1.556108	2.689222	-0.150172
23	1	0	-3.018816	2.726608	0.881130
24	1	0	-3.093103	3.330104	-0.798388
25	1	0	1.556172	2.689227	0.149376
26	1	0	3.018967	2.726492	-0.881824
27	1	0	3.093082	3.330316	0.797589
28	1	0	3.043995	-0.651841	-3.345805
29	1	0	1.515507	-0.946336	-2.466135
30	1	0	2.915637	-2.033232	-2.222155
31	1	0	4.792242	-0.386877	1.756949
32	1	0	4.932715	-1.242907	0.192042
33	1	0	4.637613	-2.166995	1.692751

$POMe_3$ – PCM (acetonitrile)

```
Zero-point correction=                           0.128940 (Hartree/Particle)
 Thermal correction to Energy=                    0.139221
 Thermal correction to Enthalpy=                  0.140165
 Thermal correction to Gibbs Free Energy=         0.092504
 Sum of electronic and zero-point Energies=           -686.647940
 Sum of electronic and thermal Energies=              -686.637660
 Sum of electronic and thermal Enthalpies=            -686.636716
 Sum of electronic and thermal Free Energies=         -686.684377
```

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

1	6	0	-1.043792	1.985003	0.643158
2	8	0	-0.834837	1.294136	-0.605959
3	6	0	2.490644	-0.442014	0.273555
4	8	0	1.392082	0.465921	0.123211
5	6	0	-1.565393	-1.972418	0.159717
6	8	0	-0.535838	-1.035032	0.504767
7	15	0	0.066608	-0.070617	-0.712193
8	1	0	-1.861809	2.689017	0.478762
9	1	0	-0.140413	2.528854	0.931211
10	1	0	-1.316799	1.281111	1.434063
11	1	0	3.342033	0.141952	0.629534
12	1	0	2.756382	-0.913980	-0.681200
13	1	0	2.253878	-1.221978	1.004984
14	1	0	-1.549514	-2.763949	0.912443
15	1	0	-1.394117	-2.416191	-0.828927
16	1	0	-2.548765	-1.489216	0.167292

TS (1Z, 2Z) – $P(OMe)_3$ – PCM (acetonitrile)

Zero-point correction= 0.508058 (Hartree/Particle)
Thermal correction to Energy= 0.548079
Thermal correction to Enthalpy= 0.549023
Thermal correction to Gibbs Free Energy= 0.426079
Sum of electronic and zero-point Energies= -2079.014021
Sum of electronic and thermal Energies= -2078.974000
Sum of electronic and thermal Enthalpies= -2078.973056
Sum of electronic and thermal Free Energies= -2079.096001

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	3.844366	-1.174493	0.203433
2	8	0	4.930040	-0.712201	1.368628
3	8	0	4.028143	-2.803315	0.441645
4	8	0	4.692037	-1.065964	-1.196724
5	6	0	6.003195	-1.650222	-1.345967
6	6	0	5.000832	0.658159	1.786904
7	6	0	3.649208	-3.363372	1.705755
8	46	0	1.726914	-0.198976	-0.056391
9	1	0	5.930674	-2.738997	-1.406275
10	1	0	6.649550	-1.370516	-0.509494
11	1	0	6.413659	-1.253831	-2.276469
12	1	0	4.006789	1.115956	1.828940
13	1	0	5.635273	1.233967	1.104047
14	1	0	5.448303	0.664310	2.783493
15	1	0	2.680256	-2.976560	2.043493
16	1	0	4.405612	-3.144624	2.465705
17	1	0	3.572132	-4.443598	1.564993
18	15	0	1.587926	2.145135	-0.111902
19	8	0	2.517897	3.101295	-1.097077
20	8	0	0.154314	2.912551	-0.432128
21	8	0	1.830803	2.764072	1.387437
22	6	0	-0.357828	2.889546	-1.770968
23	6	0	3.845158	2.696125	-1.460258
24	6	0	1.723935	4.177250	1.659908
25	1	0	-0.304728	1.883932	-2.204553
26	1	0	0.198238	3.583968	-2.408148

27	1	0	-1.403676	3.199057	-1.716233
28	1	0	4.083609	3.192709	-2.403735
29	1	0	3.910966	1.610807	-1.591418
30	1	0	4.563855	3.011984	-0.696109
31	1	0	0.678054	4.492585	1.632443
32	1	0	2.302000	4.755838	0.934247
33	1	0	2.131364	4.330206	2.660919
34	6	0	-2.055918	-2.789170	-0.474021
35	6	0	-3.340323	-2.329832	-1.112222
36	6	0	-4.531474	-2.354187	-0.134911
37	6	0	-5.848451	-1.900970	-0.801216
38	6	0	-7.011348	-2.019545	0.138262
39	6	0	-7.823503	-1.058420	0.614044
40	6	0	-0.964424	-2.039328	-0.342633
41	6	0	0.393527	-2.129344	0.189157
42	6	0	-0.492777	-0.695067	-0.672229
43	6	0	-7.756485	0.381952	0.287852
44	8	0	-6.974232	0.944726	-0.463331
45	8	0	-8.723496	1.049746	0.962099
46	6	0	-8.776274	2.469020	0.742354
47	1	0	-2.040517	-3.808494	-0.082451
48	1	0	-3.580312	-2.979188	-1.968417
49	1	0	-3.213754	-1.315766	-1.512310
50	1	0	-4.313790	-1.701512	0.720299
51	1	0	-4.651890	-3.368973	0.269336
52	1	0	-5.754115	-0.878911	-1.171273
53	1	0	-6.040694	-2.555303	-1.665441
54	1	0	-7.206738	-3.031682	0.496122
55	1	0	-8.615575	-1.328023	1.306329
56	1	0	0.502321	-2.095331	1.273681
57	1	0	1.098102	-2.783729	-0.321085
58	1	0	-0.920486	0.142649	-0.124396
59	1	0	-0.271596	-0.491819	-1.720401
60	1	0	-8.970146	2.688315	-0.310982
61	1	0	-7.835654	2.939731	1.040142
62	1	0	-9.595882	2.831289	1.362760

TS (2Z, 3Z) – P(OMe)$_3$ – PCM (acetonitrile)

Zero-point correction= 0.509656 (Hartree/Particle)
Thermal correction to Energy= 0.548670
Thermal correction to Enthalpy= 0.549614
Thermal correction to Gibbs Free Energy= 0.430821
Sum of electronic and zero-point Energies= -2079.020161
Sum of electronic and thermal Energies= -2078.981147
Sum of electronic and thermal Enthalpies= -2078.980203
Sum of electronic and thermal Free Energies= -2079.098996

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.234262	-1.974055	-1.528607
2	6	0	0.509823	-1.273348	-2.745202
3	6	0	1.382227	-2.652532	-0.957977
4	6	0	-0.833481	-1.714595	-0.627563
5	46	0	1.535837	-0.559620	-0.491163

6	6	0	-2.068156	-0.947244	-1.010416
7	6	0	-2.919053	-0.522679	0.195618
8	6	0	-4.194167	0.240268	-0.218574
9	6	0	-4.976179	0.717167	0.968828
10	6	0	-6.268048	0.506609	1.280151
11	6	0	-7.243671	-0.262813	0.479747
12	8	0	-7.057780	-0.829025	-0.586955
13	8	0	-8.446791	-0.268352	1.103654
14	6	0	-9.497772	-0.982136	0.432063
15	15	0	3.460300	-0.711206	0.707005
16	8	0	3.671696	-2.037103	1.655966
17	8	0	4.905497	-0.765533	-0.057626
18	8	0	3.732167	0.544766	1.704832
19	6	0	4.936294	0.634648	2.501854
20	6	0	2.636412	-2.414095	2.581395
21	6	0	5.079733	-1.606313	-1.210250
22	1	0	-0.266244	-0.694203	-3.233693
23	1	0	1.318288	-1.629382	-3.375522
24	1	0	2.180675	-2.978935	-1.619704
25	1	0	1.248011	-3.260453	-0.066375
26	1	0	-0.905089	-2.367747	0.240382
27	1	0	-2.704297	-1.544760	-1.692651
28	1	0	-1.794012	-0.048641	-1.579387
29	1	0	-2.311541	0.106690	0.860383
30	1	0	-3.201005	-1.410527	0.778658
31	1	0	-3.888758	1.126847	-0.797029
32	1	0	-4.818996	-0.374860	-0.868190
33	1	0	-4.403533	1.313370	1.681404
34	1	0	-6.669054	0.929136	2.196713
35	1	0	-9.233008	-2.036199	0.314173
36	1	0	-9.689770	-0.547812	-0.552692
37	1	0	-10.375595	-0.879863	1.069972
38	1	0	5.788915	0.885108	1.866332
39	1	0	5.125534	-0.306564	3.024090
40	1	0	4.762820	1.431715	3.225856
41	1	0	1.644484	-2.297741	2.130938
42	1	0	2.697814	-1.803660	3.487960
43	1	0	2.805055	-3.462493	2.833194
44	1	0	4.283207	-1.429105	-1.941393
45	1	0	5.090556	-2.662008	-0.921239
46	1	0	6.043206	-1.337847	-1.646180
47	15	0	0.938978	1.708953	-0.282782
48	8	0	1.968740	2.902125	-0.736835
49	8	0	-0.392772	2.262111	-1.058283
50	8	0	0.514050	2.080343	1.242076
51	6	0	-0.361177	2.473700	-2.481430
52	6	0	3.390711	2.714923	-0.832494
53	6	0	0.089521	3.413448	1.611365
54	1	0	0.041304	1.594456	-2.994352
55	1	0	0.243045	3.353051	-2.720391
56	1	0	-1.394614	2.637255	-2.791831
57	1	0	3.762753	3.509548	-1.482054
58	1	0	3.629495	1.741355	-1.271895
59	1	0	3.854698	2.792913	0.153681
60	1	0	-0.864313	3.653167	1.136202
61	1	0	0.844991	4.148780	1.323125
62	1	0	-0.024814	3.405374	2.695983

TS (3Z´, 4a´) – P(OMe)$_3$ – PCM (acetonitrile)

Zero-point correction= 0.381070 (Hartree/Particle)

Thermal correction to Energy=	0.406923
Thermal correction to Enthalpy=	0.407867
Thermal correction to Gibbs Free Energy=	0.324033
Sum of electronic and zero-point Energies=	-1392.347087
Sum of electronic and thermal Energies=	-1392.321234
Sum of electronic and thermal Enthalpies=	-1392.320289
Sum of electronic and thermal Free Energies=	-1392.404124

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	-0.379074	-0.484072	0.082091
2	6	0	-2.162661	-2.075526	0.335456
3	6	0	-1.106982	-2.312480	-0.669926
4	6	0	-2.881653	-0.734798	0.237913
5	6	0	-2.391564	-2.889445	1.398109
6	6	0	-2.245466	1.084357	0.630303
7	6	0	-0.822945	1.443031	0.929580
8	6	0	-3.649976	-0.457300	-1.050559
9	6	0	-0.084823	2.465752	0.188295
10	8	0	-0.247457	2.851190	-0.966319
11	8	0	0.913322	2.996001	0.969626
12	6	0	1.768818	3.946700	0.322061
13	6	0	-4.184617	0.972072	-0.942139
14	6	0	-2.987240	1.812765	-0.491962
15	1	0	-1.363618	-2.108667	-1.711781
16	1	0	-0.555112	-3.244744	-0.558726
17	1	0	-3.567566	-0.694955	1.084113
18	1	0	-3.099108	-2.624604	2.179664
19	1	0	-1.875090	-3.841011	1.497055
20	1	0	-2.801928	1.105443	1.566795
21	1	0	-0.577389	1.439041	1.988909
22	1	0	-4.459027	-1.191812	-1.161868
23	1	0	-2.998332	-0.554905	-1.927429
24	1	0	1.193773	4.795319	-0.058288
25	1	0	2.310529	3.482013	-0.506764
26	1	0	2.469866	4.280687	1.088229
27	1	0	-4.603922	1.335023	-1.886950
28	1	0	-4.986624	1.009342	-0.191935
29	1	0	-3.294772	2.803036	-0.130360
30	1	0	-2.306947	1.978827	-1.328353
31	15	0	1.817182	-0.683889	-0.256148
32	8	0	2.791254	-0.629465	1.051563
33	8	0	2.441930	-2.012780	-0.960971
34	8	0	2.366640	0.445115	-1.277661
35	6	0	2.509061	-3.255899	-0.237849
36	6	0	2.417963	0.094913	2.243514
37	6	0	3.764316	0.513513	-1.654538
38	1	0	1.551877	-3.485593	0.240161
39	1	0	3.296290	-3.209804	0.518774
40	1	0	2.742142	-4.027116	-0.973248
41	1	0	3.275566	0.026818	2.914604
42	1	0	1.545606	-0.369613	2.712641
43	1	0	2.200235	1.140254	2.014863
44	1	0	4.033412	-0.352914	-2.262091
45	1	0	4.397442	0.560125	-0.765071
46	1	0	3.873453	1.429033	-2.236362

TS (2Z,6) – P(OMe)$_3$ – PCM (acetonitrile)

Zero-point correction= 0.511662 (Hartree/Particle)
Thermal correction to Energy= 0.549211
Thermal correction to Enthalpy= 0.550155
Thermal correction to Gibbs Free Energy= 0.439874
Sum of electronic and zero-point Energies= -2079.024465
Sum of electronic and thermal Energies= -2078.986916
Sum of electronic and thermal Enthalpies= -2078.985972
Sum of electronic and thermal Free Energies= -2079.096253

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.821918	-1.731921	0.325710
2	8	0	2.205890	-1.672168	1.911912
3	8	0	1.598165	-3.348198	0.215714
4	8	0	3.226529	-1.609294	-0.478609
5	6	0	4.367604	-2.439428	-0.153303
6	6	0	2.158811	-0.438509	2.663534
7	6	0	0.610265	-3.996342	1.036706
8	46	0	0.192239	-0.328849	-0.675966
9	6	0	-1.930561	-1.045663	-1.792952
10	6	0	-1.391241	0.278606	-2.046016
11	6	0	-3.214965	-1.342695	-1.286821
12	6	0	-0.821954	-1.963430	-1.685843
13	6	0	-4.446017	-0.531152	-1.636960
14	6	0	-5.437903	-0.695524	-0.478868
15	6	0	-4.653674	-0.375622	0.795852
16	6	0	-3.294224	-1.070939	0.794025
17	6	0	-2.171829	-0.522289	1.461770
18	6	0	-2.011933	0.840443	1.849277
19	8	0	-2.697002	1.835672	1.559983
20	8	0	-0.937044	0.992706	2.724009
21	6	0	-0.750708	2.303738	3.257996
22	1	0	4.175426	-3.474143	-0.444995
23	1	0	4.586458	-2.386790	0.916083
24	1	0	5.205893	-2.038417	-0.723880
25	1	0	1.179436	0.035444	2.563958
26	1	0	2.942749	0.244089	2.328723
27	1	0	2.330923	-0.719022	3.704302
28	1	0	-0.361985	-3.499239	0.950917
29	1	0	0.928421	-4.001836	2.082374
30	1	0	0.526461	-5.019874	0.668165
31	1	0	-2.013414	1.147217	-1.845832
32	1	0	-0.755402	0.392130	-2.925944
33	1	0	-3.412237	-2.415719	-1.258711
34	1	0	-0.990036	-2.937756	-1.231821
35	1	0	-0.090362	-1.975870	-2.497382
36	1	0	-4.892852	-0.856423	-2.588629
37	1	0	-4.191349	0.530429	-1.752698
38	1	0	-5.798800	-1.734208	-0.454824
39	1	0	-6.319377	-0.051538	-0.588008
40	1	0	-4.499303	0.701824	0.879727
41	1	0	-5.208861	-0.696126	1.689820
42	1	0	-3.370802	-2.149593	0.932345
43	1	0	-1.411722	-1.203725	1.831087
44	1	0	-1.656156	2.660801	3.758785
45	1	0	-0.470493	3.018008	2.478666
46	1	0	0.061214	2.214388	3.983545
47	15	0	1.191005	1.818508	-0.546294
48	8	0	1.625089	2.381314	-2.028352

49	8	0	0.429078	3.158114	-0.023086
50	8	0	2.544505	1.913809	0.345824
51	6	0	-0.840173	3.573413	-0.574448
52	6	0	2.335930	1.528946	-2.945154
53	6	0	3.306968	3.139504	0.458197
54	1	0	-1.642239	2.962798	-0.153114
55	1	0	-0.826019	3.520056	-1.666443
56	1	0	-0.972412	4.613132	-0.268739
57	1	0	2.385197	2.068237	-3.892400
58	1	0	1.810415	0.579742	-3.092149
59	1	0	3.349987	1.333120	-2.582699
60	1	0	2.778755	3.850822	1.096685
61	1	0	3.478475	3.578998	-0.527452
62	1	0	4.259122	2.863298	0.912628

TS (7Z,5a) – $P(OMe)_3$ – PCM (acetonitrile)

Zero-point correction= 0.511927 (Hartree/Particle)
Thermal correction to Energy= 0.549744
Thermal correction to Enthalpy= 0.550688
Thermal correction to Gibbs Free Energy= 0.437429
Sum of electronic and zero-point Energies= -2079.028243
Sum of electronic and thermal Energies= -2078.990427
Sum of electronic and thermal Enthalpies= -2078.989483
Sum of electronic and thermal Free Energies= -2079.102742

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.105474	-1.397162	0.020947
2	15	0	0.972058	2.117786	-0.343701
3	8	0	2.504719	-2.246346	1.374857
4	8	0	2.212261	-2.613682	-1.059858
5	8	0	3.422642	-0.459701	-0.239965
6	8	0	1.651277	2.495279	-1.805554
7	8	0	0.075383	3.491326	-0.171918
8	8	0	2.134412	2.485273	0.743535
9	6	0	4.767053	-0.982563	-0.279656
10	6	0	2.383613	-1.603602	2.655816
11	6	0	2.905478	-3.866286	-0.869744
12	6	0	-1.042252	3.701824	-1.052823
13	6	0	2.034883	1.459966	-2.724858
14	6	0	2.827976	3.750930	0.731010
15	46	0	0.114894	-0.251510	0.051868
16	6	0	-2.220895	-2.205503	0.369687
17	6	0	-0.817555	-2.284033	0.135204
18	6	0	-3.245416	-1.922069	-0.705979
19	6	0	-2.756853	-2.185589	1.646739
20	6	0	-2.764030	-1.502480	-2.108872
21	6	0	-3.900607	-0.611972	-2.640025
22	6	0	-4.288914	0.234527	-1.415790
23	6	0	-4.220413	-0.744775	-0.210190
24	6	0	-3.829666	-0.165136	1.131234
25	6	0	-2.713598	0.656103	1.303101
26	8	0	-1.830729	0.891117	0.424023
27	8	0	-2.587277	1.195388	2.569556

28	6	0	-1.429442	1.992225	2.810167
29	1	0	4.944043	-1.492536	-1.231150
30	1	0	4.944620	-1.668637	0.552930
31	1	0	5.437527	-0.125737	-0.196574
32	1	0	1.402871	-1.125601	2.758981
33	1	0	3.171359	-0.855230	2.789774
34	1	0	2.491607	-2.386139	3.408604
35	1	0	2.553598	-4.365155	0.035180
36	1	0	3.986615	-3.716022	-0.810126
37	1	0	2.670581	-4.473328	-1.745439
38	1	0	-1.754703	2.877243	-0.967374
39	1	0	-0.702750	3.806727	-2.088288
40	1	0	-1.517017	4.631966	-0.733408
41	1	0	2.127278	1.931512	-3.705722
42	1	0	1.275060	0.671824	-2.772685
43	1	0	2.991979	1.018697	-2.434471
44	1	0	2.153646	4.558944	1.024755
45	1	0	3.238074	3.953738	-0.262111
46	1	0	3.640521	3.663974	1.454258
47	1	0	-0.507275	-2.594418	-0.862559
48	1	0	-0.246858	-2.780105	0.920038
49	1	0	-3.873253	-2.816894	-0.823946
50	1	0	-2.114041	-2.212400	2.525787
51	1	0	-3.789633	-2.467214	1.822079
52	1	0	-2.553998	-2.360013	-2.759314
53	1	0	-1.843366	-0.910569	-2.031394
54	1	0	-4.747584	-1.235939	-2.959028
55	1	0	-3.601322	-0.004499	-3.502698
56	1	0	-3.553872	1.032213	-1.278944
57	1	0	-5.276874	0.699982	-1.512392
58	1	0	-5.215456	-1.186556	-0.081152
59	1	0	-4.572404	-0.141581	1.922776
60	1	0	-1.312228	2.777231	2.057929
61	1	0	-0.518636	1.380637	2.815282
62	1	0	-1.573915	2.435366	3.798267

TS (7E,5b) – $P(OMe)_3$ – PCM (acetonitrile)

Zero-point correction= 0.511912 (Hartree/Particle)
Thermal correction to Energy= 0.549747
Thermal correction to Enthalpy= 0.550691
Thermal correction to Gibbs Free Energy= 0.437528
Sum of electronic and zero-point Energies= -2079.031862
Sum of electronic and thermal Energies= -2078.994026
Sum of electronic and thermal Enthalpies= -2078.993082
Sum of electronic and thermal Free Energies= -2079.106246

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.958975	-1.757469	0.015556
2	8	0	3.001455	-1.808655	1.283795
3	8	0	1.721718	-3.374581	-0.164699
4	8	0	2.912126	-1.510688	-1.284360
5	6	0	4.110577	-2.287886	-1.507301
6	6	0	3.012772	-0.777974	2.289286
7	6	0	1.461336	-4.217707	0.969845

8	15	0	1.577967	1.880250	-0.412801
9	8	0	1.706167	2.249556	-2.019960
10	8	0	1.238687	3.397838	0.130141
11	8	0	3.129188	1.799972	0.101466
12	6	0	0.062819	4.082265	-0.345031
13	6	0	1.518340	1.219609	-3.006576
14	6	0	4.098525	2.826719	-0.201312
15	46	0	0.219265	-0.252132	0.082525
16	6	0	-2.562247	-1.564786	-0.005811
17	6	0	-1.204901	-1.951992	-0.213718
18	6	0	-3.350581	-0.808476	-1.048074
19	6	0	-3.170524	-1.639929	1.232456
20	6	0	-4.572191	-1.558288	-1.645666
21	6	0	-5.625682	-0.466703	-1.892914
22	6	0	-5.495206	0.420523	-0.646864
23	6	0	-3.973318	0.518261	-0.388345
24	6	0	-3.604194	0.701541	1.060298
25	6	0	-2.324126	1.141196	1.386443
26	8	0	-1.386454	1.281881	0.539491
27	8	0	-2.096155	1.394287	2.722568
28	6	0	-0.778421	1.808563	3.076262
29	1	0	3.864571	-3.347104	-1.611081
30	1	0	4.813499	-2.147537	-0.681943
31	1	0	4.547869	-1.913483	-2.433748
32	1	0	1.993385	-0.532833	2.605187
33	1	0	3.500454	0.122091	1.909625
34	1	0	3.570051	-1.182342	3.136366
35	1	0	0.714384	-3.777714	1.639877
36	1	0	2.382478	-4.397401	1.529797
37	1	0	1.076808	-5.159174	0.573399
38	1	0	-0.433607	2.640898	2.455977
39	1	0	-0.824840	3.459785	-0.208737
40	1	0	0.179271	4.350656	-1.399080
41	1	0	-0.026653	4.990759	0.254234
42	1	0	1.466107	1.723310	-3.973937
43	1	0	0.585887	0.671876	-2.829604
44	1	0	2.354106	0.514645	-3.000380
45	1	0	3.845236	3.754270	0.317385
46	1	0	4.143031	3.005431	-1.278888
47	1	0	5.061212	2.453307	0.151385
48	1	0	-0.907821	-2.112049	-1.252991
49	1	0	-0.839194	-2.732084	0.448108
50	1	0	-2.683696	-0.520027	-1.868192
51	1	0	-2.628542	-1.997011	2.106747
52	1	0	-4.250181	-1.626776	1.330849
53	1	0	-4.960439	-2.278872	-0.913625
54	1	0	-4.310689	-2.122604	-2.548079
55	1	0	-6.635857	-0.867709	-2.035405
56	1	0	-5.369465	0.108219	-2.793684
57	1	0	-5.962602	1.405291	-0.762695
58	1	0	-5.988288	-0.072136	0.203295
59	1	0	-3.571205	1.361185	-0.964222
60	1	0	-4.382183	0.775963	1.813877
61	1	0	-0.062073	0.983490	2.974234
62	1	0	-0.833034	2.115543	4.123038

TS (4a,5a) – $P(OMe)_3$ – PCM (acetonitrile)

Zero-point correction=	0.512392 (Hartree/Particle)
Thermal correction to Energy=	0.550477
Thermal correction to Enthalpy=	0.551421
Thermal correction to Gibbs Free Energy=	0.436530
Sum of electronic and zero-point Energies=	-2079.023168
Sum of electronic and thermal Energies=	-2078.985083
Sum of electronic and thermal Enthalpies=	-2078.984139
Sum of electronic and thermal Free Energies=	-2079.099030

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.323972	-0.103011	-0.179120
2	15	0	2.530126	-1.073891	-0.174596
3	15	0	-0.105086	2.180631	-0.397305
4	8	0	3.704563	-0.582291	0.886566
5	8	0	2.750142	-2.696299	0.038004
6	8	0	3.238210	-0.951501	-1.648944
7	8	0	0.674353	3.024343	-1.594099
8	8	0	-1.599500	2.814526	-0.717355
9	8	0	0.219496	3.036607	0.961953
10	6	0	4.538150	-1.515414	-1.925779
11	6	0	3.773223	0.794300	1.287802
12	6	0	2.449572	-3.278262	1.318724
13	6	0	-2.245590	2.451798	-1.945145
14	6	0	2.048048	2.749315	-1.899837
15	6	0	0.018791	4.464073	1.034879
16	1	0	4.476544	-2.605039	-1.979596
17	1	0	5.257283	-1.224724	-1.155029
18	1	0	4.850204	-1.112865	-2.891047
19	1	0	2.772632	1.221097	1.419429
20	1	0	4.322976	1.382785	0.545170
21	1	0	4.309204	0.822259	2.239021
22	1	0	1.593590	-2.786553	1.792781
23	1	0	3.319683	-3.199169	1.978605
24	1	0	2.220849	-4.332098	1.143894
25	1	0	-2.227962	1.365228	-2.097411
26	1	0	-1.763777	2.946569	-2.794426
27	1	0	-3.282511	2.785411	-1.867811
28	1	0	2.252730	3.208894	-2.869489
29	1	0	2.235755	1.672185	-1.958072
30	1	0	2.708761	3.191827	-1.145766
31	1	0	-1.047646	4.695535	1.092955
32	1	0	0.456756	4.962663	0.165994
33	1	0	0.520928	4.799810	1.943972
34	6	0	-2.199592	-1.950408	-1.525389
35	6	0	-2.554194	-1.568519	-2.763164
36	6	0	-3.152176	-2.415383	-0.443985
37	6	0	-0.785102	-1.915511	-1.091084
38	6	0	-4.643693	-2.132967	-0.663256
39	6	0	-4.815073	-0.629235	-0.328861
40	6	0	-3.598092	-0.242998	0.562212
41	6	0	-2.806496	-1.555390	0.798461
42	6	0	-1.297366	-1.503509	0.995230
43	6	0	-0.744637	-0.660292	2.107522
44	8	0	0.257319	-0.960125	2.756605
45	8	0	-1.522271	0.394562	2.449499
46	6	0	-1.062460	1.185706	3.557824
47	1	0	-3.583732	-1.596938	-3.107354
48	1	0	-1.813199	-1.229996	-3.483536

49	1	0	-2.959925	-3.479536	-0.242916
50	1	0	-0.137863	-1.479079	-1.865509
51	1	0	-0.380565	-2.876276	-0.777829
52	1	0	-5.218387	-2.746048	0.041403
53	1	0	-4.996407	-2.393890	-1.666406
54	1	0	-5.768308	-0.442212	0.176852
55	1	0	-4.820249	-0.029288	-1.244865
56	1	0	-2.962904	0.491096	0.059712
57	1	0	-3.904496	0.205798	1.509141
58	1	0	-3.225591	-2.056398	1.685126
59	1	0	-0.904682	-2.499929	1.179372
60	1	0	-0.139552	1.705760	3.292477
61	1	0	-0.899220	0.560324	4.438742
62	1	0	-1.857610	1.907795	3.745686

TS (2Z,4a) – $P(OMe)_3$ – PCM (acetonitrile)

Zero-point correction= 0.511316 (Hartree/Particle)
Thermal correction to Energy= 0.549121
Thermal correction to Enthalpy= 0.550065
Thermal correction to Gibbs Free Energy= 0.438356
Sum of electronic and zero-point Energies= -2079.022007
Sum of electronic and thermal Energies= -2078.984202
Sum of electronic and thermal Enthalpies= -2078.983258
Sum of electronic and thermal Free Energies= -2079.094967

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	46	0	0.244849	-0.342285	-0.656092
2	6	0	-1.775030	-1.274027	-1.785304
3	6	0	-1.355427	0.078219	-2.088895
4	6	0	-3.030433	-1.664350	-1.262749
5	6	0	-0.591893	-2.089130	-1.640595
6	6	0	-4.329730	-0.972699	-1.623368
7	6	0	-5.296038	-1.196857	-0.453141
8	6	0	-4.535717	-0.772824	0.806656
9	6	0	-3.126114	-1.358515	0.808572
10	6	0	-2.022853	-0.754004	1.464351
11	6	0	-1.827688	0.581140	1.928467
12	8	0	-0.909965	0.949068	2.684853
13	8	0	-2.773908	1.513718	1.530510
14	6	0	-2.710034	2.776001	2.199168
15	15	0	2.025355	-1.527666	0.366121
16	15	0	1.030106	1.887584	-0.478045
17	8	0	2.271646	-1.581709	1.977110
18	8	0	2.122226	-3.134436	0.078938
19	8	0	3.434070	-1.056805	-0.290964
20	8	0	1.621596	2.440169	-1.907986
21	8	0	0.096802	3.176351	-0.127315
22	8	0	2.222553	2.130004	0.594822
23	6	0	4.688655	-1.687610	0.061005
24	6	0	2.070963	-0.425510	2.826447
25	6	0	1.295804	-4.061202	0.806071
26	6	0	-1.096046	3.463741	-0.881489
27	6	0	2.462548	1.598561	-2.718788
28	6	0	2.861009	3.419014	0.756533

29	1	0	-2.064344	0.893008	-1.965528
30	1	0	-0.690861	0.210348	-2.944834
31	1	0	-3.134927	-2.749325	-1.210227
32	1	0	-0.684590	-3.058994	-1.156271
33	1	0	0.143611	-2.069383	-2.447921
34	1	0	-4.752695	-1.356810	-2.563930
35	1	0	-4.172199	0.104753	-1.763836
36	1	0	-5.560788	-2.262955	-0.399188
37	1	0	-6.233060	-0.638529	-0.570686
38	1	0	-4.483383	0.315623	0.854073
39	1	0	-5.057483	-1.110602	1.714146
40	1	0	-3.135075	-2.438487	0.958085
41	1	0	-1.221205	-1.413929	1.784801
42	1	0	-1.762335	3.284896	2.006179
43	1	0	-2.831415	2.656403	3.281015
44	1	0	4.731030	-2.698009	-0.351457
45	1	0	4.809387	-1.722459	1.146585
46	1	0	5.471917	-1.069733	-0.379446
47	1	0	1.040800	-0.064347	2.757264
48	1	0	2.769664	0.370095	2.556007
49	1	0	2.282051	-0.769079	3.841077
50	1	0	0.244150	-3.756709	0.785831
51	1	0	1.633511	-4.139143	1.842329
52	1	0	1.401795	-5.025322	0.306233
53	1	0	-1.883993	2.753472	-0.620254
54	1	0	-0.894837	3.438824	-1.956120
55	1	0	-1.402139	4.470943	-0.593961
56	1	0	2.562244	2.099460	-3.683094
57	1	0	2.011113	0.611463	-2.862033
58	1	0	3.449246	1.484224	-2.259963
59	1	0	2.184972	4.110541	1.263781
60	1	0	3.154671	3.827997	-0.213371
61	1	0	3.746196	3.243483	1.368895
62	1	0	-3.538030	3.364054	1.797526