Electronic Supplementary Material (ESI) for Dalton Transactions.

DFT supporting information for:

DFT examination of rare α-$SiMe_3$ abstraction in $Ta(NMe_2)_4[N(SiMe_3)_2]$: Formation of the imide compound $Ta(=NSiMe_3)(NMe_2)_3$ and its trapping to give guanidinate imides

Michael G. Richmond*[,a] and Zi-Ling Xue[b]

1) M06 geometries and energies for all optimized minima and transition structures (S2-S31)
2) B3LYP geometries and energies for all optimized minima and transition structures (S32-S61)
3) The complete list of authors for ref. 29 (S62)

1) M06 geometries and energies for all optimized minima and transition structures (S2-S31)

Species A1
HF energy = -1468.03096128
No imaginary frequency
Zero-point correction = 0.559983 (Hartree/Particle)
Thermal correction to Energy = 0.594742
Thermal correction to Enthalpy = 0.595686
Thermal correction to Gibbs Free Energy = 0.499851
Sum of electronic and zero-point Energies = -1467.470978
Sum of electronic and thermal Energies = -1467.436220
Sum of electronic and thermal Enthalpies = -1467.435276
Sum of electronic and thermal Free Energies = -1467.531111

Coordinates: **A1**

Ta	7.09050000	5.22370000	3.55960000
N	6.24800000	6.84790000	2.65140000
N	8.06850000	5.89770000	5.17040000
N	5.21870000	4.94810000	4.42190000
N	8.62790000	5.43420000	2.18440000
N	7.22110000	3.15390000	3.43300000
C	6.89110000	8.14380000	2.70360000
H	7.03820000	8.58010000	1.69560000
H	6.27330000	8.86100000	3.28010000
H	7.87710000	8.08920000	3.18520000
C	4.98810000	6.94010000	1.95690000
H	4.36480000	7.75930000	2.36550000
H	5.13130000	7.15270000	0.87770000
H	4.41740000	6.00550000	2.04030000
C	4.33510000	3.80460000	4.42530000
H	3.94290000	3.60160000	5.44100000
H	3.45270000	3.97640000	3.77460000
H	4.85730000	2.90750000	4.07710000
C	4.49800000	6.07570000	4.98590000
H	3.54100000	6.26120000	4.46040000
H	4.24460000	5.87930000	6.04600000
H	5.09160000	6.99980000	4.94550000
C	7.58490000	5.78650000	6.53840000
H	8.29340000	5.20860000	7.16110000
H	7.47890000	6.78640000	6.99710000
H	6.61170000	5.28470000	6.57030000
C	9.31950000	6.63820000	5.14980000
H	10.09790000	6.11930000	5.74010000
H	9.69150000	6.76490000	4.12700000
H	9.18270000	7.63960000	5.59780000
C	8.66060000	6.12850000	0.91760000
H	7.70590000	6.62950000	0.71840000
H	9.46580000	6.88960000	0.89190000

H	8.86220000	5.42810000	0.08250000
C	9.87720000	4.71640000	2.35400000
H	10.07260000	4.02650000	1.51110000
H	10.73340000	5.41830000	2.39740000
H	9.88470000	4.12310000	3.27680000
Si	6.78190000	2.44730000	1.89380000
Si	7.78480000	2.14480000	4.75160000
C	6.56590000	2.05540000	6.18910000
H	6.28020000	3.04120000	6.58190000
H	5.64220000	1.53440000	5.89710000
H	7.02130000	1.48290000	7.01190000
C	9.44900000	2.70960000	5.44270000
H	9.48360000	3.77930000	5.68840000
H	9.66760000	2.14200000	6.36050000
H	10.26040000	2.49730000	4.72960000
C	8.08530000	0.34780000	4.24310000
H	8.67740000	0.23530000	3.32360000
H	8.65930000	-0.12500000	5.05560000
H	7.15730000	-0.22690000	4.12580000
C	5.68530000	0.90950000	2.04900000
H	5.05780000	0.91400000	2.95240000
H	5.00740000	0.87080000	1.18240000
H	6.26560000	-0.02280000	2.04820000
C	8.28200000	1.98110000	0.84480000
H	9.12820000	1.64500000	1.46170000
H	8.02880000	1.16850000	0.14740000
H	8.62950000	2.83510000	0.24490000
C	5.74530000	3.67370000	0.89520000
H	4.74540000	3.80940000	1.33460000
H	6.20290000	4.66500000	0.75420000
H	5.60180000	3.24670000	-0.11020000

Species A2

HF energy = -1468.02328151
No imaginary frequency
Zero-point correction = 0.560357 (Hartree/Particle)
Thermal correction to Energy = 0.594906
Thermal correction to Enthalpy = 0.595850
Thermal correction to Gibbs Free Energy = 0.500255
Sum of electronic and zero-point Energies = -1467.462925
Sum of electronic and thermal Energies = -1467.428375
Sum of electronic and thermal Enthalpies = -1467.427431
Sum of electronic and thermal Free Energies = -1467.523026

Coordinates: **A2**

Ta	7.06430000	5.19140000	3.59640000
N	5.84420000	5.94980000	2.08120000
N	8.12990000	5.77790000	5.29180000

N	5.39270000	5.37630000	4.76310000
N	8.61950000	6.02880000	2.56070000
N	7.26810000	3.21830000	3.33130000
C	4.39250000	5.88260000	2.06140000
H	3.93100000	6.88790000	2.12830000
H	4.03760000	5.44070000	1.10930000
H	4.00240000	5.26900000	2.88060000
C	6.24230000	6.73690000	0.92730000
H	5.74180000	6.37530000	0.00930000
H	5.95450000	7.80090000	1.04170000
H	7.32060000	6.68630000	0.75790000
C	4.70620000	4.26830000	5.39000000
H	4.75580000	4.31690000	6.49760000
H	3.63030000	4.26740000	5.11980000
H	5.12690000	3.30490000	5.06850000
C	4.75480000	6.63010000	5.08570000
H	3.70580000	6.65530000	4.73250000
H	4.73070000	6.81510000	6.17700000
H	5.28670000	7.47330000	4.61810000
C	7.60170000	6.13340000	6.59710000
H	8.19600000	5.66630000	7.40490000
H	7.64570000	7.22730000	6.76910000
H	6.56590000	5.80640000	6.71640000
C	9.56130000	6.02250000	5.33910000
H	10.03130000	5.42790000	6.14720000
H	10.05090000	5.75220000	4.39780000
H	9.79200000	7.08310000	5.56300000
C	8.95440000	7.43250000	2.59630000
H	8.24900000	7.98910000	3.23310000
H	9.97340000	7.59950000	2.99580000
H	8.92550000	7.89060000	1.58880000
C	9.52220000	5.30390000	1.69430000
H	9.46270000	5.65510000	0.64310000
H	10.57550000	5.43870000	2.01520000
H	9.30900000	4.22560000	1.70410000
Si	6.63560000	2.39290000	1.87870000
Si	8.04910000	2.15740000	4.53740000
C	8.07180000	2.81650000	6.29610000
H	8.80630000	3.61690000	6.43760000
H	7.09470000	3.18250000	6.64090000
H	8.35550000	1.97180000	6.94490000
C	9.84540000	1.87520000	4.05250000
H	10.37400000	2.84080000	4.02210000
H	10.34770000	1.25130000	4.80710000
H	9.97500000	1.39370000	3.07460000
C	7.10440000	0.52970000	4.73010000
H	6.91310000	-0.05370000	3.82210000
H	7.68190000	-0.10980000	5.41590000

H	6.13570000	0.72120000	5.21790000
C	4.89340000	1.78230000	2.24000000
H	4.24680000	2.64280000	2.47520000
H	4.46760000	1.28330000	1.35660000
H	4.84030000	1.08230000	3.08420000
C	7.78750000	0.99540000	1.33670000
H	8.06430000	0.24880000	2.08890000
H	7.29920000	0.46200000	0.50620000
H	8.71700000	1.42610000	0.93230000
C	6.53640000	3.44780000	0.32660000
H	5.66750000	4.11510000	0.32520000
H	7.43380000	4.05740000	0.15280000
H	6.43820000	2.75550000	-0.52510000

Species A3

HF energy = -1468.01949035
No imaginary frequency
Zero-point correction = 0.558422 (Hartree/Particle)
Thermal correction to Energy = 0.594109
Thermal correction to Enthalpy = 0.595054
Thermal correction to Gibbs Free Energy = 0.495803
Sum of electronic and zero-point Energies = -1467.461069
Sum of electronic and thermal Energies = -1467.425381
Sum of electronic and thermal Enthalpies = -1467.424437
Sum of electronic and thermal Free Energies = -1467.523687

Coordinates: **A3**

Ta	7.10250000	5.12020000	3.53580000
N	7.06130000	7.21820000	3.58420000
N	7.42100000	5.10590000	5.52810000
N	5.16240000	5.17640000	3.04960000
N	8.61500000	5.35950000	2.22200000
N	7.21800000	3.00450000	3.38220000
C	8.06780000	8.18060000	3.20190000
H	7.71710000	8.86040000	2.39720000
H	8.34580000	8.82850000	4.05670000
H	8.98300000	7.68520000	2.85610000
C	5.99920000	7.91770000	4.28090000
H	6.38180000	8.44680000	5.17580000
H	5.52300000	8.68760000	3.63980000
H	5.21170000	7.22500000	4.61150000
C	4.22280000	4.18770000	3.54690000
H	3.43370000	4.67210000	4.15260000
H	3.72290000	3.65730000	2.71370000
H	4.72360000	3.43200000	4.16540000
C	4.50110000	6.12290000	2.17450000
H	4.06980000	5.61220000	1.29460000
H	3.67220000	6.63400000	2.69850000

H	5.20780000	6.88570000	1.82430000
C	6.38110000	5.10020000	6.53080000
H	6.69450000	4.53100000	7.42700000
H	6.13270000	6.12790000	6.86180000
H	5.45660000	4.64190000	6.15010000
C	8.58240000	5.83840000	5.98520000
H	9.00110000	5.38960000	6.90540000
H	9.38620000	5.83890000	5.23060000
H	8.33510000	6.89660000	6.20070000
C	8.59070000	6.02900000	0.94500000
H	7.61910000	6.51650000	0.77750000
H	9.37040000	6.81110000	0.87290000
H	8.76620000	5.31600000	0.11640000
C	9.92570000	4.84870000	2.55350000
H	10.31890000	4.19450000	1.75330000
H	10.65550000	5.66880000	2.70700000
H	9.89690000	4.24270000	3.47210000
Si	7.00630000	2.32110000	1.78090000
Si	7.67360000	1.90070000	4.66660000
C	6.30780000	1.66850000	5.94990000
H	6.09320000	2.55180000	6.56210000
H	5.37250000	1.35710000	5.45870000
H	6.59680000	0.85530000	6.63400000
C	9.29140000	2.35530000	5.52720000
H	9.29620000	3.35530000	5.97660000
H	9.48160000	1.62470000	6.32880000
H	10.13550000	2.28100000	4.82310000
C	8.00000000	0.11860000	4.09610000
H	8.64670000	0.01610000	3.21400000
H	8.51410000	-0.38690000	4.92930000
H	7.07470000	-0.44090000	3.90470000
C	5.88290000	0.79070000	1.77150000
H	5.19280000	0.77840000	2.62870000
H	5.26760000	0.80260000	0.85890000
H	6.43930000	-0.15540000	1.77850000
C	8.66980000	1.89650000	0.98090000
H	9.41200000	1.52170000	1.70110000
H	8.54500000	1.13430000	0.19670000
H	9.09630000	2.79250000	0.50470000
C	6.14110000	3.46750000	0.54860000
H	5.07950000	3.60810000	0.79680000
H	6.59530000	4.45740000	0.41060000
H	6.17980000	2.95750000	-0.42840000

Species TSA2BC
HF energy = -1467.98751007
Imaginary frequency: 140*i*
Zero-point correction = 0.559049 (Hartree/Particle)

Thermal correction to Energy = 0.593132
Thermal correction to Enthalpy = 0.594077
Thermal correction to Gibbs Free Energy = 0.499264
Sum of electronic and zero-point Energies = -1467.428461
Sum of electronic and thermal Energies = -1467.394378
Sum of electronic and thermal Enthalpies = -1467.393433
Sum of electronic and thermal Free Energies = -1467.488246

Coordinates: **TSA2BC**

Ta	8.11020000	5.47410000	4.34260000
N	7.39160000	5.95130000	6.15350000
N	6.19440000	5.04860000	3.67940000
N	8.39150000	6.68280000	2.75510000
N	8.98470000	3.74810000	4.36730000
C	5.15840000	4.53060000	4.55430000
H	4.34880000	5.27360000	4.69610000
H	4.68730000	3.62260000	4.13280000
H	5.55920000	4.26550000	5.54160000
C	5.62460000	5.25940000	2.36700000
H	5.26420000	4.31010000	1.92250000
H	4.74800000	5.93580000	2.41480000
H	6.35750000	5.70080000	1.68010000
C	6.59730000	7.13800000	6.37520000
H	5.61790000	6.88270000	6.82180000
H	7.10550000	7.84380000	7.05950000
H	6.39630000	7.66850000	5.43240000
C	7.51740000	5.16880000	7.36480000
H	6.51690000	4.92660000	7.77120000
H	8.03570000	4.21830000	7.17740000
H	8.06760000	5.71540000	8.15490000
C	7.79340000	7.99780000	2.70030000
H	7.23540000	8.22430000	3.62220000
H	8.56400000	8.78270000	2.58400000
H	7.08590000	8.09190000	1.85390000
C	9.10260000	6.37360000	1.53290000
H	8.41940000	6.38000000	0.66130000
H	9.90030000	7.11150000	1.33090000
H	9.56530000	5.37910000	1.58650000
Si	8.50120000	2.31990000	3.44100000
C	6.92270000	1.55090000	4.13020000
H	6.83970000	1.69140000	5.21810000
H	6.03580000	2.00550000	3.66550000
H	6.89120000	0.47060000	3.92610000
C	9.82960000	0.98420000	3.31900000
H	10.10280000	0.50720000	4.26790000
H	9.42990000	0.20010000	2.65600000
H	10.75000000	1.36220000	2.85320000
C	8.21570000	2.79790000	1.63740000

H	9.14970000	3.15860000	1.17850000
H	7.90450000	1.90400000	1.07440000
H	7.44110000	3.56400000	1.49550000
Si	10.44880000	3.76360000	5.59470000
N	10.18140000	5.92980000	5.07000000
C	11.15230000	6.27420000	4.04090000
H	11.16720000	5.53070000	3.23370000
H	10.92550000	7.26260000	3.59420000
H	12.17470000	6.33040000	4.46080000
C	10.24590000	6.99620000	6.06370000
H	9.86040000	7.95010000	5.64240000
H	9.64810000	6.76160000	6.95130000
H	11.28300000	7.19250000	6.39020000
C	11.24750000	4.43620000	7.20970000
H	10.53380000	4.81570000	7.95610000
H	11.77700000	3.59270000	7.68090000
H	11.98270000	5.23000000	7.01530000
C	9.83630000	2.15520000	6.49940000
H	9.15850000	1.47770000	5.96410000
H	10.71750000	1.56530000	6.80370000
H	9.33010000	2.43260000	7.43970000
C	11.95740000	3.32980000	4.52850000
H	12.32270000	2.33570000	4.82800000
H	11.74380000	3.29220000	3.45110000
H	12.77980000	4.04080000	4.68740000

Species B

HF energy = -924.395561450
No imaginary frequency
Zero-point correction = 0.360518 (Hartree/Particle)
Thermal correction to Energy = 0.385516
Thermal correction to Enthalpy = 0.386460
Thermal correction to Gibbs Free Energy = 0.306041
Sum of electronic and zero-point Energies = -924.035044
Sum of electronic and thermal Energies = -924.010046
Sum of electronic and thermal Enthalpies = -924.009102
Sum of electronic and thermal Free Energies = -924.089520

Coordinates: **B**

Ta	6.94340000	5.23010000	3.71860000
N	7.81110000	5.69170000	5.48120000
N	4.95300000	5.54190000	3.80820000
N	7.76520000	6.31560000	2.23260000
N	7.24110000	3.49330000	3.37920000
C	3.92120000	4.53630000	3.95540000
H	3.29060000	4.73900000	4.84100000
H	3.25400000	4.51470000	3.07330000
H	4.36740000	3.54080000	4.07250000

C	4.38550000	6.86050000	3.62590000
H	3.70850000	6.89100000	2.75180000
H	3.80260000	7.17940000	4.51080000
H	5.16730000	7.61800000	3.45270000
C	7.39850000	6.83980000	6.25930000
H	7.04550000	6.53920000	7.26370000
H	8.22740000	7.55930000	6.39970000
H	6.56700000	7.37850000	5.77690000
C	8.82880000	4.92350000	6.16740000
H	8.46350000	4.55660000	7.14530000
H	9.12730000	4.05540000	5.56630000
H	9.73000000	5.53480000	6.36110000
C	8.01340000	7.73160000	2.39980000
H	7.69390000	8.08450000	3.39430000
H	9.08980000	7.96780000	2.30530000
H	7.47180000	8.33210000	1.64450000
C	8.25870000	5.83600000	0.95870000
H	7.75420000	6.34530000	0.11660000
H	9.34410000	6.02320000	0.85410000
H	8.08650000	4.75700000	0.86070000
Si	7.51960000	1.81360000	3.08570000
C	8.77510000	1.15730000	4.32570000
H	9.74150000	1.67040000	4.21600000
H	8.42610000	1.31830000	5.35600000
H	8.95090000	0.07980000	4.19390000
C	8.18310000	1.58230000	1.33900000
H	9.12300000	2.13610000	1.20070000
H	8.38180000	0.52350000	1.11760000
H	7.46340000	1.95100000	0.59390000
C	5.90280000	0.86550000	3.27090000
H	5.14600000	1.24250000	2.56780000
H	6.03720000	-0.20860000	3.07620000
H	5.49810000	0.97320000	4.28770000

Species C

HF energy = -543.607263076
No imaginary frequency
Zero-point correction = 0.193313 (Hartree/Particle)
Thermal correction to Energy = 0.205030
Thermal correction to Enthalpy = 0.205975
Thermal correction to Gibbs Free Energy = 0.157103
Sum of electronic and zero-point Energies = -543.413950
Sum of electronic and thermal Energies = -543.402233
Sum of electronic and thermal Enthalpies = -543.401288
Sum of electronic and thermal Free Energies = -543.450160

Coordinates: **C**

Si	-0.85820000	0.84880000	0.06730000

N	-0.22460000	1.75150000	-1.29180000
C	1.19260000	1.67250000	-1.57300000
H	1.55660000	0.64090000	-1.46970000
H	1.39540000	1.98990000	-2.61000000
H	1.80480000	2.31950000	-0.90950000
C	-0.72340000	3.09310000	-1.50740000
H	-0.52200000	3.41590000	-2.54290000
H	-1.81140000	3.13660000	-1.35730000
H	-0.25540000	3.84290000	-0.83490000
C	-0.32430000	1.63010000	1.69960000
H	-0.70720000	2.65750000	1.79110000
H	-0.68550000	1.06350000	2.56980000
H	0.77280000	1.68050000	1.76980000
C	-2.73430000	0.84030000	-0.03810000
H	-3.07260000	0.52320000	-1.03420000
H	-3.15010000	0.13560000	0.69650000
H	-3.17700000	1.82380000	0.17250000
C	-0.20000000	-0.90940000	-0.02310000
H	-0.74640000	-1.55270000	0.68150000
H	-0.32740000	-1.33330000	-1.02880000
H	0.86480000	-0.97260000	0.24060000

Species D

HF energy = -1848.85459433
No imaginary frequency
Zero-point correction = 0.729147 (Hartree/Particle)
Thermal correction to Energy = 0.775799
Thermal correction to Enthalpy = 0.776743
Thermal correction to Gibbs Free Energy = 0.656193
Sum of electronic and zero-point Energies = -1848.125447
Sum of electronic and thermal Energies = -1848.078796
Sum of electronic and thermal Enthalpies = -1848.077852
Sum of electronic and thermal Free Energies = -1848.198401

Coordinates: **D**

Ta	26.13160000	15.91540000	14.59390000
Ta	25.33020000	13.71200000	12.42870000
N	26.44480000	17.96220000	14.71390000
N	24.39700000	16.21350000	15.62530000
N	27.86460000	15.56620000	15.53770000
N	23.84610000	14.61830000	11.35770000
N	26.86900000	12.82900000	11.50190000
N	24.21390000	11.96640000	12.32360000
N	26.17860000	15.69330000	12.64950000
N	25.50090000	13.85800000	14.37440000
Si	26.89120000	16.68000000	11.40380000
Si	25.37760000	12.66240000	15.63590000
C	25.39990000	18.96220000	14.62060000

H	25.31940000	19.55010000	15.55710000
H	24.42290000	18.49920000	14.42090000
H	25.60020000	19.68610000	13.81000000
C	27.71430000	18.63240000	14.89980000
H	27.92740000	19.33910000	14.07330000
H	28.54390000	17.91420000	14.94800000
H	27.72060000	19.23020000	15.83480000
C	24.30550000	17.03940000	16.81180000
H	23.55130000	17.84150000	16.69360000
H	25.26710000	17.51840000	17.04150000
H	24.00160000	16.43710000	17.68970000
C	23.09460000	15.66930000	15.31180000
H	22.67820000	15.11300000	16.17530000
H	23.13800000	14.97860000	14.45960000
H	22.37270000	16.47360000	15.06630000
C	28.16010000	15.98030000	16.89180000
H	28.44570000	15.11690000	17.52070000
H	27.29100000	16.46280000	17.36230000
H	29.00120000	16.69870000	16.91570000
C	28.99270000	14.89510000	14.92900000
H	29.90720000	15.51520000	15.00040000
H	28.80770000	14.70210000	13.86390000
H	29.20170000	13.92890000	15.42900000
C	23.23500000	15.90240000	11.62390000
H	23.25940000	16.54690000	10.72270000
H	23.75640000	16.43540000	12.43030000
H	22.17050000	15.78970000	11.91100000
C	23.23770000	14.02600000	10.18350000
H	22.13680000	13.96200000	10.28140000
H	23.61520000	13.00980000	10.00640000
H	23.44730000	14.63400000	9.28180000
C	26.82150000	12.36690000	10.13140000
H	27.63910000	12.80900000	9.53290000
H	25.87140000	12.63920000	9.64850000
H	26.92910000	11.26710000	10.07580000
C	28.13770000	12.51800000	12.12420000
H	28.37610000	11.44200000	12.01800000
H	28.11570000	12.74580000	13.19790000
H	28.96380000	13.09040000	11.65940000
C	24.72560000	10.62590000	12.13470000
H	24.41730000	9.95150000	12.95810000
H	25.82280000	10.61820000	12.09030000
H	24.33890000	10.17610000	11.19660000
C	22.76920000	11.90640000	12.41820000
H	22.31980000	11.51400000	11.48380000
H	22.34170000	12.90060000	12.61260000
H	22.44040000	11.23420000	13.23150000
C	28.75750000	16.77270000	11.67530000

H	29.00550000	17.24970000	12.63630000
H	29.24730000	17.35170000	10.87760000
H	29.19900000	15.76330000	11.67270000
C	26.63310000	15.92420000	9.69460000
H	27.14570000	14.95520000	9.60510000
H	27.05120000	16.59360000	8.92730000
H	25.56860000	15.76880000	9.46450000
C	26.21300000	18.43800000	11.33680000
H	25.11930000	18.46610000	11.44770000
H	26.46410000	18.89610000	10.36830000
H	26.64730000	19.06450000	12.12750000
C	25.67340000	13.42420000	17.33680000
H	26.70550000	13.79010000	17.43900000
H	25.51280000	12.66440000	18.11680000
H	24.99280000	14.26520000	17.53820000
C	23.70730000	11.79420000	15.70860000
H	22.86710000	12.49590000	15.60760000
H	23.60000000	11.27840000	16.67490000
H	23.61610000	11.04220000	14.91420000
C	26.71130000	11.34850000	15.39320000
H	26.60280000	10.83410000	14.42620000
H	26.66120000	10.58500000	16.18450000
H	27.71720000	11.79670000	15.42850000

Species E

HF energy = -227.228081304
No imaginary frequency
Zero-point correction = 0.089994 (Hartree/Particle)
Thermal correction to Energy = 0.096693
Thermal correction to Enthalpy = 0.097637
Thermal correction to Gibbs Free Energy = 0.059263
Sum of electronic and zero-point Energies = -227.138088
Sum of electronic and thermal Energies = -227.131388
Sum of electronic and thermal Enthalpies = -227.130444
Sum of electronic and thermal Free Energies = -227.168818

Coordinates: **E**

C	-0.91860000	0.22750000	-0.40520000
N	0.18400000	-0.15160000	-0.77000000
N	-2.08350000	0.50490000	-0.16440000
C	1.28460000	-0.59140000	0.05570000
H	1.54720000	-1.62400000	-0.20950000
H	2.16570000	0.03170000	-0.14580000
H	1.06510000	-0.55350000	1.13250000
C	-2.65200000	1.81050000	0.07720000
H	-3.42780000	2.01250000	-0.67290000
H	-3.13810000	1.82200000	1.06150000
H	-1.91170000	2.62270000	0.04090000

Species TSBEF
HF energy = -1151.63191760
Imaginary frequency: 256*i*
Zero-point correction = 0.452377 (Hartree/Particle)
Thermal correction to Energy = 0.483501
Thermal correction to Enthalpy = 0.484445
Thermal correction to Gibbs Free Energy = 0.391846
Sum of electronic and zero-point Energies = -1151.179540
Sum of electronic and thermal Energies = -1151.148417
Sum of electronic and thermal Enthalpies = -1151.147473
Sum of electronic and thermal Free Energies = -1151.240072

Coordinates: **TSBEF**

Ta	6.40510000	5.12510000	4.27770000
N	7.51350000	6.14780000	5.78960000
N	4.62760000	5.42490000	3.32300000
N	7.57040000	5.80450000	2.75380000
N	6.87810000	3.39220000	4.37510000
C	4.23310000	4.63130000	2.18110000
H	3.17650000	4.30950000	2.25670000
H	4.33950000	5.19900000	1.23430000
H	4.85480000	3.72790000	2.10060000
C	3.75530000	6.55550000	3.51580000
H	3.76560000	7.23850000	2.64180000
H	2.70070000	6.24650000	3.66190000
H	4.05470000	7.14280000	4.39910000
C	7.65480000	7.56790000	5.55470000
H	7.82680000	8.12280000	6.49710000
H	8.49200000	7.79780000	4.86490000
H	6.73400000	7.98350000	5.10510000
C	8.74560000	5.56370000	6.28410000
H	9.11650000	6.10060000	7.17770000
H	8.58500000	4.50870000	6.54860000
H	9.55670000	5.60090000	5.52810000
C	7.22940000	6.93460000	1.91950000
H	6.19870000	7.27150000	2.10860000
H	7.90440000	7.79710000	2.08960000
H	7.30360000	6.67460000	0.84580000
C	8.90490000	5.33280000	2.45810000
H	9.00390000	5.05750000	1.38970000
H	9.67000000	6.10880000	2.66310000
H	9.14840000	4.44710000	3.06160000
Si	7.28730000	1.76350000	3.98980000
C	8.84950000	1.29180000	4.93110000
H	9.68030000	1.95620000	4.64890000
H	8.69510000	1.39810000	6.01470000
H	9.16470000	0.25700000	4.73370000

C	7.59890000	1.61300000	2.13660000
H	8.45420000	2.23300000	1.83080000
H	7.81080000	0.57610000	1.83710000
H	6.72240000	1.95620000	1.56650000
C	5.86670000	0.62440000	4.47130000
H	4.94790000	0.92560000	3.94590000
H	6.07210000	-0.42570000	4.21720000
H	5.66490000	0.67790000	5.55060000
C	5.74130000	5.92420000	7.10610000
N	5.12200000	5.33360000	6.16590000
N	5.85950000	6.52230000	8.15860000
C	3.86800000	4.64170000	6.46150000
H	4.00700000	3.56220000	6.30780000
H	3.53460000	4.82610000	7.49140000
H	3.09700000	4.98720000	5.76150000
C	6.86830000	6.51550000	9.18170000
H	6.40860000	6.77600000	10.14200000
H	7.35890000	5.53670000	9.28020000
H	7.63440000	7.27280000	8.96400000

Species F

HF energy = -1151.67695063
No imaginary frequency
Zero-point correction = 0.456729 (Hartree/Particle)
Thermal correction to Energy = 0.487012
Thermal correction to Enthalpy = 0.487956
Thermal correction to Gibbs Free Energy = 0.397682
Sum of electronic and zero-point Energies = -1151.220221
Sum of electronic and thermal Energies = -1151.189939
Sum of electronic and thermal Enthalpies = -1151.188995
Sum of electronic and thermal Free Energies = -1151.279269

Coordinates: **F**

Ta	6.23360000	5.21610000	3.98660000
N	7.33120000	5.76400000	6.08960000
N	4.58480000	5.18000000	2.83370000
N	7.50420000	6.51760000	3.07920000
N	6.94060000	3.57370000	3.82560000
C	4.03530000	4.08070000	2.07110000
H	3.03930000	3.78700000	2.45530000
H	3.90690000	4.35760000	1.00800000
H	4.69740000	3.20810000	2.12170000
C	3.74460000	6.35500000	2.73600000
H	3.73250000	6.76490000	1.70900000
H	2.69830000	6.12630000	3.01610000
H	4.08620000	7.15510000	3.41320000
C	7.83810000	7.14010000	6.13480000
H	8.20100000	7.41230000	7.13830000

H	8.66100000	7.24250000	5.41430000
H	7.03620000	7.83410000	5.85160000
C	8.35870000	4.79740000	6.49290000
H	8.85220000	5.08110000	7.43520000
H	7.89750000	3.80880000	6.61010000
H	9.11660000	4.73400000	5.69830000
C	7.14050000	7.89490000	2.84210000
H	6.14010000	8.12380000	3.24630000
H	7.85130000	8.59900000	3.32040000
H	7.11990000	8.13380000	1.76180000
C	8.83880000	6.23550000	2.60090000
H	8.93530000	6.45320000	1.52010000
H	9.59850000	6.85560000	3.12110000
H	9.09180000	5.17880000	2.75800000
Si	7.53670000	1.95160000	3.79960000
C	9.40680000	1.99610000	3.57180000
H	9.67770000	2.48570000	2.62520000
H	9.88700000	2.55680000	4.38810000
H	9.84050000	0.98550000	3.56300000
C	6.74480000	1.01980000	2.36870000
H	6.92140000	1.53860000	1.41570000
H	7.14980000	0.00120000	2.27880000
H	5.65710000	0.93480000	2.50740000
C	7.13270000	1.06170000	5.41030000
H	6.05800000	1.12620000	5.63200000
H	7.40330000	-0.00320000	5.35820000
H	7.67490000	1.49670000	6.26260000
C	6.02330000	5.61790000	6.77860000
N	5.11680000	5.51520000	5.77140000
N	5.76370000	5.57830000	8.02320000
C	3.73340000	5.32040000	6.14440000
H	3.13820000	5.13310000	5.24170000
H	3.62680000	4.46570000	6.82990000
H	3.33330000	6.20350000	6.66720000
C	6.76350000	5.69410000	9.05030000
H	7.63170000	6.32860000	8.80120000
H	6.30350000	6.12180000	9.95180000
H	7.15350000	4.70330000	9.33960000

Species TSFG1
HF energy = -1151.64926321
Imaginary frequency: 82*i*
Zero-point correction = 0.455833 (Hartree/Particle)
Thermal correction to Energy = 0.485778
Thermal correction to Enthalpy = 0.486722
Thermal correction to Gibbs Free Energy = 0.396577
Sum of electronic and zero-point Energies = -1151.193430

Sum of electronic and thermal Energies = -1151.163486
Sum of electronic and thermal Enthalpies = -1151.162541
Sum of electronic and thermal Free Energies = -1151.252687

Coordinates: **TSFG1**

Ta	6.09520000	5.34700000	3.94510000
N	7.53750000	5.40120000	7.27250000
N	4.19140000	4.87950000	3.53890000
N	6.78990000	6.28130000	2.31310000
N	7.08400000	3.85670000	4.17480000
C	3.59170000	3.58270000	3.32000000
H	2.98780000	3.26990000	4.19270000
H	2.92320000	3.59590000	2.44000000
H	4.36880000	2.82600000	3.15030000
C	3.20260000	5.90900000	3.78140000
H	2.53950000	6.04460000	2.90700000
H	2.57600000	5.67310000	4.66070000
H	3.68160000	6.88450000	3.98320000
C	8.79280000	6.08130000	7.01530000
H	9.47590000	5.87590000	7.85200000
H	9.26400000	5.73150000	6.07840000
H	8.64480000	7.16310000	6.94420000
C	7.72870000	3.99880000	7.59730000
H	8.11950000	3.87710000	8.61880000
H	6.79540000	3.43940000	7.50270000
H	8.44890000	3.55090000	6.88800000
C	5.97880000	6.98220000	1.34220000
H	4.91280000	6.93090000	1.60630000
H	6.26430000	8.04890000	1.27540000
H	6.09230000	6.54470000	0.33240000
C	8.19360000	6.29530000	1.95800000
H	8.36450000	5.82500000	0.97110000
H	8.58050000	7.32970000	1.90650000
H	8.78790000	5.75190000	2.70620000
Si	8.07150000	2.48060000	3.84570000
C	9.88280000	2.85640000	4.21170000
H	10.21860000	3.73980000	3.64830000
H	10.05210000	3.06070000	5.27920000
H	10.53000000	2.01350000	3.92730000
C	7.90190000	2.03910000	2.02140000
H	8.22740000	2.88020000	1.39120000
H	8.50090000	1.15870000	1.74610000
H	6.85210000	1.82630000	1.77010000
C	7.50830000	1.01990000	4.89210000
H	6.44250000	0.81120000	4.71890000
H	8.07370000	0.10830000	4.64960000
H	7.63780000	1.21910000	5.96550000
C	6.41680000	5.80650000	6.56850000

N	6.65960000	6.64450000	5.45490000
N	5.18900000	5.45120000	6.76770000
C	6.09750000	7.98520000	5.53650000
H	6.09980000	8.44460000	4.53560000
H	5.06450000	7.99080000	5.92650000
H	6.70940000	8.63340000	6.18870000
C	4.78750000	4.72430000	7.94710000
H	5.47560000	4.85050000	8.80120000
H	3.79340000	5.07710000	8.25650000
H	4.68460000	3.64450000	7.74690000

Species G1

HF energy = -1151.68665648
No imaginary frequency
Zero-point correction = 0.456965 (Hartree/Particle)
Thermal correction to Energy = 0.487465
Thermal correction to Enthalpy = 0.488409
Thermal correction to Gibbs Free Energy = 0.397086
Sum of electronic and zero-point Energies = -1151.229691
Sum of electronic and thermal Energies = -1151.199191
Sum of electronic and thermal Enthalpies = -1151.198247
Sum of electronic and thermal Free Energies = -1151.289571

Coordinates: **G1**

Ta	5.51210000	3.05370000	11.13840000
Si	4.31610000	3.28400000	14.37360000
N	5.20540000	3.12640000	12.90420000
N	5.76420000	1.06930000	10.76580000
N	3.59950000	2.89190000	10.02370000
N	4.52430000	4.86510000	10.31690000
N	2.32900000	4.81290000	9.35570000
C	2.83170000	4.40750000	14.06200000
H	3.16910000	5.39300000	13.70820000
H	2.21990000	4.56130000	14.96300000
H	2.18200000	3.97640000	13.28380000
C	3.70360000	1.58750000	14.91720000
H	3.11740000	1.12030000	14.11100000
H	3.06660000	1.64170000	15.81200000
H	4.54590000	0.91810000	15.14380000
C	5.40170000	4.03350000	15.71580000
H	6.27710000	3.39820000	15.91060000
H	4.85560000	4.15530000	16.66260000
H	5.77100000	5.02270000	15.40970000
C	5.77900000	-0.00920000	11.72640000
H	4.87710000	-0.65000000	11.63110000
H	5.81250000	0.38410000	12.74950000
H	6.65690000	-0.66800000	11.58120000
C	5.73460000	0.56330000	9.41520000

H	6.63890000	-0.02900000	9.17780000
H	5.66930000	1.38100000	8.67940000
H	4.85600000	-0.09270000	9.24130000
C	3.44420000	4.21840000	9.87900000
C	1.50230000	4.14690000	8.37250000
H	2.04990000	3.31110000	7.92580000
H	1.25740000	4.85770000	7.56840000
H	0.55660000	3.77150000	8.79700000
C	1.88010000	6.12080000	9.78380000
H	2.38540000	6.40770000	10.71080000
H	0.79970000	6.08010000	9.99100000
H	2.05390000	6.89820000	9.02190000
C	2.49750000	1.99150000	10.28510000
H	1.66160000	2.49170000	10.80410000
H	2.09640000	1.51830000	9.37320000
H	2.86080000	1.18220000	10.93590000
C	4.93650000	6.17400000	9.87670000
H	4.60050000	6.39440000	8.84950000
H	4.57510000	6.98420000	10.53180000
H	6.03470000	6.21570000	9.89260000
N	7.32680000	3.88940000	10.81320000
C	8.22270000	4.53890000	11.73800000
H	8.38630000	5.60180000	11.46650000
H	7.81240000	4.50310000	12.75490000
H	9.21710000	4.05200000	11.75030000
C	7.83340000	3.89930000	9.46310000
H	7.10210000	3.46610000	8.75630000
H	8.04650000	4.92810000	9.10780000
H	8.76780000	3.31400000	9.36450000

Species TSG1G2
HF energy = -1151.67859811
Imaginary frequency: 25*i*
Zero-point correction = 0.456391 (Hartree/Particle)
Thermal correction to Energy = 0.486419
Thermal correction to Enthalpy = 0.487363
Thermal correction to Gibbs Free Energy = 0.395887
Sum of electronic and zero-point Energies = -1151.222208
Sum of electronic and thermal Energies = -1151.192179
Sum of electronic and thermal Enthalpies = -1151.191235
Sum of electronic and thermal Free Energies = -1151.282711

Coordinates: **TSG1G2**

Ta	5.19080000	2.45820000	10.88360000
Si	4.14650000	3.06070000	14.17390000
N	4.50270000	2.59080000	12.55020000
N	5.76040000	0.54390000	10.76560000
N	3.56620000	2.82720000	9.72160000

N	6.58870000	3.32990000	9.19680000
N	6.97740000	3.62460000	11.36270000
N	8.62720000	4.41940000	9.82720000
C	5.12460000	4.60720000	14.63190000
H	6.19900000	4.38660000	14.71230000
H	4.79530000	5.03120000	15.59190000
H	5.00210000	5.37940000	13.85810000
C	2.30780000	3.42460000	14.37210000
H	2.01470000	4.32310000	13.81030000
H	2.04980000	3.59520000	15.42780000
H	1.69700000	2.58690000	14.00660000
C	4.62280000	1.66410000	15.34890000
H	4.07370000	0.74250000	15.10750000
H	4.40470000	1.92070000	16.39610000
H	5.69790000	1.43980000	15.27660000
C	5.69750000	-0.46560000	11.80350000
H	4.98260000	-1.26720000	11.53970000
H	5.38280000	-0.01880000	12.75370000
H	6.68530000	-0.94110000	11.94680000
C	6.16340000	-0.03250000	9.49590000
H	7.14440000	-0.53370000	9.58820000
H	6.26410000	0.74330000	8.72280000
H	5.43470000	-0.78620000	9.14340000
C	7.43020000	3.80560000	10.10760000
C	9.46160000	4.00810000	8.72060000
H	9.06340000	3.09300000	8.27080000
H	10.47810000	3.79160000	9.08780000
H	9.54100000	4.78470000	7.94180000
C	9.16370000	5.46840000	10.66550000
H	8.38100000	5.86200000	11.32200000
H	9.51690000	6.29450000	10.02840000
H	10.01230000	5.12830000	11.28280000
C	3.50310000	2.46600000	8.32130000
H	2.74960000	1.67280000	8.15170000
H	3.21470000	3.32630000	7.68580000
H	4.46740000	2.08640000	7.95460000
C	6.53610000	3.88750000	7.86530000
H	6.88850000	3.17690000	7.09690000
H	5.49800000	4.14820000	7.61210000
H	7.13460000	4.80740000	7.77230000
C	7.87010000	3.45040000	12.48930000
H	8.84410000	3.03280000	12.18360000
H	8.05870000	4.38680000	13.04010000
H	7.41230000	2.74480000	13.19830000
C	2.26100000	3.26100000	10.17860000
H	2.28240000	3.49760000	11.24800000
H	1.92470000	4.16040000	9.62840000
H	1.49790000	2.47570000	10.01350000

Species G2
HF energy = -1151.67991773
No imaginary frequency
Zero-point correction = 0.456499 (Hartree/Particle)
Thermal correction to Energy = 0.487485
Thermal correction to Enthalpy = 0.488429
Thermal correction to Gibbs Free Energy = 0.395218
Sum of electronic and zero-point Energies = -1151.223418
Sum of electronic and thermal Energies = -1151.192433
Sum of electronic and thermal Enthalpies = -1151.191489
Sum of electronic and thermal Free Energies = -1151.284700

Coordinates: **G2**

Ta	5.29870000	2.46560000	10.94440000
Si	4.20830000	2.81250000	14.28050000
N	4.71840000	2.56860000	12.64890000
N	5.40360000	0.46270000	10.67230000
N	3.79560000	3.33000000	9.92210000
N	6.93560000	2.84840000	9.19490000
N	7.01520000	3.71620000	11.24460000
N	8.70830000	4.38230000	9.69710000
C	4.27770000	4.64620000	14.71120000
H	5.29930000	5.03890000	14.60190000
H	3.95480000	4.83490000	15.74550000
H	3.62640000	5.23060000	14.04490000
C	2.43480000	2.19770000	14.43700000
H	1.78680000	2.72380000	13.72050000
H	2.02300000	2.35040000	15.44510000
H	2.37600000	1.12410000	14.20560000
C	5.31510000	1.85290000	15.46650000
H	5.33160000	0.78510000	15.20440000
H	4.96810000	1.93930000	16.50660000
H	6.35170000	2.21860000	15.42900000
C	4.93790000	-0.54310000	11.61060000
H	4.11890000	-1.14430000	11.17210000
H	4.56830000	-0.07570000	12.53040000
H	5.75110000	-1.24570000	11.87300000
C	5.86310000	-0.18200000	9.45660000
H	6.65460000	-0.92210000	9.67840000
H	6.28000000	0.54740000	8.75170000
H	5.03910000	-0.72620000	8.95640000
C	7.58510000	3.65420000	10.01820000
C	9.73630000	3.86400000	8.82320000
H	9.60290000	2.78690000	8.68160000
H	10.72140000	4.02080000	9.29140000
H	9.74770000	4.35610000	7.83610000
C	8.93050000	5.71550000	10.21160000

H	8.02200000	6.08660000	10.69610000
H	9.17050000	6.39400000	9.37740000
H	9.76330000	5.75570000	10.93370000
C	3.54750000	3.00510000	8.53390000
H	2.54200000	2.56270000	8.40240000
H	3.60620000	3.90050000	7.88600000
H	4.27560000	2.27050000	8.15900000
C	7.06930000	2.99150000	7.76420000
H	7.81020000	2.29890000	7.32810000
H	6.10820000	2.76520000	7.28020000
H	7.35070000	4.01420000	7.46200000
C	7.75600000	4.06810000	12.43580000
H	8.83030000	3.84620000	12.32880000
H	7.65510000	5.13270000	12.70490000
H	7.36870000	3.48260000	13.28000000
C	2.73230000	4.14750000	10.46630000
H	2.92220000	4.37520000	11.52240000
H	2.64580000	5.10380000	9.91730000
H	1.75370000	3.63550000	10.39050000

Species TSG1EH
HF energy = -1378.90032157
Imaginary frequency: 290*i*
Zero-point correction = 0.548112 (Hartree/Particle)
Thermal correction to Energy = 0.585093
Thermal correction to Enthalpy = 0.586037
Thermal correction to Gibbs Free Energy = 0.481212
Sum of electronic and zero-point Energies = -1378.352210
Sum of electronic and thermal Energies = -1378.315229
Sum of electronic and thermal Enthalpies = -1378.314284
Sum of electronic and thermal Free Energies = -1378.419110

Coordinates: **TSG1EH**

Ta	5.66430000	4.25040000	11.73330000
Si	3.73820000	3.04360000	14.30030000
N	5.00890000	3.57490000	13.28070000
N	7.64410000	3.80190000	11.48190000
N	5.42200000	2.38670000	10.51640000
N	3.85140000	3.91470000	10.48920000
N	3.25220000	1.72570000	9.72540000
C	3.32960000	1.24280000	13.89980000
H	3.08320000	1.14160000	12.83010000
H	2.47300000	0.86990000	14.48080000
H	4.19010000	0.58880000	14.10290000
C	4.19060000	3.17300000	16.12680000
H	5.13540000	2.65300000	16.34030000
H	3.41160000	2.72800000	16.76360000
H	4.30800000	4.22250000	16.43370000

C	2.19350000	4.08380000	13.98630000
H	2.39230000	5.14440000	14.20070000
H	1.33520000	3.76840000	14.59770000
H	1.90300000	4.01270000	12.92650000
C	8.58070000	3.50510000	12.53660000
H	9.01190000	2.48960000	12.41930000
H	8.09310000	3.54330000	13.51890000
H	9.43300000	4.21610000	12.54700000
C	8.20960000	3.52400000	10.18610000
H	9.10230000	4.15140000	9.99390000
H	7.48530000	3.71760000	9.38110000
H	8.52620000	2.46450000	10.08710000
C	4.14490000	2.64410000	10.21590000
C	3.67760000	0.61170000	8.90720000
H	4.66290000	0.81620000	8.47610000
H	2.96500000	0.48560000	8.07760000
H	3.72090000	-0.33650000	9.46900000
C	1.85330000	1.73480000	10.09730000
H	1.67670000	2.47420000	10.88560000
H	1.57320000	0.74630000	10.49610000
H	1.19540000	1.95780000	9.24120000
C	5.85950000	1.07620000	10.95000000
H	5.07320000	0.53060000	11.49990000
H	6.20140000	0.44100000	10.11640000
H	6.71150000	1.20420000	11.63170000
C	2.79460000	4.64670000	9.84070000
H	2.37530000	4.08610000	8.99120000
H	1.96790000	4.89780000	10.52780000
H	3.18400000	5.59420000	9.44350000
N	5.38860000	6.30220000	11.07720000
C	4.31460000	7.16940000	11.51920000
H	3.42960000	7.12050000	10.85920000
H	3.99120000	6.88320000	12.53140000
H	4.64600000	8.22510000	11.54590000
C	5.85920000	6.66440000	9.76390000
H	6.61330000	5.94400000	9.40330000
H	5.05220000	6.71470000	9.00750000
H	6.34550000	7.66170000	9.80000000
C	6.86090000	6.89610000	12.47430000
N	6.60620000	5.88180000	13.18940000
N	7.32570000	7.98220000	12.14320000
C	7.07910000	5.85650000	14.56860000
H	6.55000000	5.04540000	15.08510000
H	8.16100000	5.66310000	14.62870000
H	6.86900000	6.80870000	15.07700000
C	8.71810000	8.23840000	11.84550000
H	8.85000000	8.40640000	10.76690000
H	9.04500000	9.14950000	12.36300000

H	9.37390000	7.40640000	12.14890000

Species H
HF energy = -1378.96879889
No imaginary frequency
Zero-point correction = 0.553125 (Hartree/Particle)
Thermal correction to Energy = 0.589130
Thermal correction to Enthalpy = 0.590075
Thermal correction to Gibbs Free Energy = 0.487828
Sum of electronic and zero-point Energies = -1378.415674
Sum of electronic and thermal Energies = -1378.379668
Sum of electronic and thermal Enthalpies = -1378.378724
Sum of electronic and thermal Free Energies = -1378.480971

Coordinates: **H**

Ta	5.86990000	3.94680000	11.95820000
Si	4.62940000	2.73550000	15.01260000
N	5.36850000	3.29850000	13.56080000
N	7.68570000	3.04030000	11.76970000
N	5.03260000	2.58720000	10.44610000
N	3.88270000	4.37830000	11.01880000
N	2.78150000	2.75800000	9.63810000
C	4.58860000	0.85190000	14.97750000
H	4.01090000	0.49460000	14.11240000
H	4.14430000	0.42040000	15.88600000
H	5.61010000	0.45480000	14.87810000
C	5.60170000	3.30400000	16.52330000
H	6.64450000	2.95850000	16.47090000
H	5.16680000	2.91370000	17.45520000
H	5.61800000	4.40100000	16.59720000
C	2.87890000	3.43060000	15.09250000
H	2.91460000	4.53040000	15.10810000
H	2.32140000	3.09680000	15.97940000
H	2.31110000	3.13170000	14.19840000
C	8.34380000	2.28370000	12.81720000
H	8.26700000	1.19210000	12.63220000
H	7.89650000	2.49840000	13.79450000
H	9.42230000	2.52650000	12.86590000
C	8.29560000	2.73800000	10.49460000
H	9.35510000	3.05740000	10.45840000
H	7.75790000	3.22180000	9.66770000
H	8.28160000	1.64680000	10.29670000
C	3.85470000	3.23610000	10.34350000
C	2.95670000	1.90570000	8.48310000
H	3.98560000	1.98200000	8.11690000
H	2.28330000	2.24460000	7.68080000
H	2.72830000	0.84830000	8.69780000
C	1.41590000	2.96910000	10.06720000

H	1.39980000	3.44680000	11.05130000
H	0.90440000	1.99690000	10.15450000
H	0.84730000	3.59180000	9.35750000
C	5.09940000	1.13930000	10.47950000
H	4.17440000	0.68980000	10.88020000
H	5.29730000	0.68960000	9.49230000
H	5.92530000	0.84500000	11.14360000
C	2.98380000	5.48650000	10.81790000
H	2.48400000	5.44160000	9.83620000
H	2.20550000	5.54160000	11.59730000
H	3.54990000	6.42950000	10.85770000
N	6.70590000	5.75550000	10.35920000
C	6.17800000	5.89680000	9.00250000
H	6.62070000	5.11050000	8.37490000
H	5.08930000	5.76720000	9.00990000
H	6.41150000	6.88470000	8.57790000
C	8.15870000	5.98330000	10.34800000
H	8.56410000	5.81940000	11.35360000
H	8.63780000	5.27840000	9.65750000
H	8.37630000	7.01390000	10.02150000
C	6.11080000	6.69670000	11.32550000
N	5.98430000	5.99180000	12.48630000
N	5.84710000	7.87150000	10.90520000
C	5.59440000	6.59770000	13.74510000
H	5.96420000	5.96450000	14.56140000
H	6.02560000	7.60000000	13.87280000
H	4.49790000	6.66750000	13.85580000
C	5.16830000	8.86700000	11.69900000
H	4.66190000	9.57160000	11.02420000
H	4.40570000	8.46580000	12.38680000
H	5.87670000	9.46370000	12.29710000

Species TSHI
HF energy = -1378.93426213
Imaginary frequency: 125*i*
Zero-point correction = 0.552488 (Hartree/Particle)
Thermal correction to Energy = 0.588098
Thermal correction to Enthalpy = 0.589042
Thermal correction to Gibbs Free Energy = 0.487036
Sum of electronic and zero-point Energies = -1378.381774
Sum of electronic and thermal Energies = -1378.346164
Sum of electronic and thermal Enthalpies = -1378.345220
Sum of electronic and thermal Free Energies = -1378.447226

Coordinates: **TSHI**

Ta	5.67020000	3.91550000	12.03420000
Si	4.02270000	3.13340000	15.04560000
N	4.80620000	3.53050000	13.56440000

N	7.33180000	2.78970000	12.37020000
N	5.16000000	2.30670000	10.63150000
N	4.14740000	4.24280000	10.41740000
N	3.31510000	2.41850000	9.10280000
C	4.00940000	1.25630000	15.23280000
H	3.45120000	0.79300000	14.40600000
H	3.54440000	0.93660000	16.17720000
H	5.03340000	0.85500000	15.20630000
C	4.94080000	3.88450000	16.51200000
H	5.99180000	3.56000000	16.52770000
H	4.48400000	3.58680000	17.46750000
H	4.93530000	4.98270000	16.46330000
C	2.24350000	3.75550000	15.04470000
H	2.20000000	4.84850000	14.93610000
H	1.72430000	3.48810000	15.97700000
H	1.68060000	3.31810000	14.20790000
C	7.69030000	2.05400000	13.55780000
H	7.60490000	0.95670000	13.40510000
H	7.04320000	2.33620000	14.39650000
H	8.74020000	2.25220000	13.85040000
C	8.20000000	2.44480000	11.27080000
H	9.26150000	2.66370000	11.50060000
H	7.93290000	2.99970000	10.35730000
H	8.13540000	1.36530000	11.02080000
C	4.17150000	2.97820000	10.01320000
C	3.72260000	1.31790000	8.25670000
H	4.81490000	1.27720000	8.19450000
H	3.33260000	1.48440000	7.24110000
H	3.34670000	0.34410000	8.61270000
C	1.92380000	2.80950000	9.01540000
H	1.63020000	3.36280000	9.91270000
H	1.30080000	1.90330000	8.96590000
H	1.70820000	3.42440000	8.12630000
C	5.06310000	0.89550000	10.93880000
H	4.02260000	0.57950000	11.12750000
H	5.47860000	0.24950000	10.14760000
H	5.63980000	0.70330000	11.85370000
C	3.50560000	5.31180000	9.69180000
H	3.66600000	5.22160000	8.60300000
H	2.42010000	5.36630000	9.87130000
H	3.92130000	6.26220000	10.04240000
N	6.19930000	7.43430000	10.52540000
C	5.37420000	8.62290000	10.50070000
H	4.59930000	8.55620000	9.71820000
H	4.87720000	8.73350000	11.46860000
H	5.99370000	9.50890000	10.29370000
C	6.89350000	7.11720000	9.29560000
H	7.06460000	6.03500000	9.23190000

H	6.26360000	7.41110000	8.44120000
H	7.86140000	7.63460000	9.20120000
C	6.09230000	6.53130000	11.55210000
N	7.02510000	5.57270000	11.73060000
N	4.97620000	6.46370000	12.27970000
C	8.44450000	5.77040000	11.53150000
H	8.98590000	5.22660000	12.31830000
H	8.81870000	5.40110000	10.56130000
H	8.70590000	6.83730000	11.60490000
C	5.11430000	6.61550000	13.72000000
H	4.27820000	6.11800000	14.22690000
H	6.05160000	6.20440000	14.14320000
H	5.06790000	7.68770000	13.98870000

Species I

HF energy = -1378.97517351
No imaginary frequency
Zero-point correction = 0.552723 (Hartree/Particle)
Thermal correction to Energy = 0.589248
Thermal correction to Enthalpy = 0.590192
Thermal correction to Gibbs Free Energy = 0.485903
Sum of electronic and zero-point Energies = -1378.422450
Sum of electronic and thermal Energies = -1378.385926
Sum of electronic and thermal Enthalpies = -1378.384982
Sum of electronic and thermal Free Energies = -1378.489271

Coordinates: **I**

Ta	5.29310000	2.73730000	11.06470000
Si	4.04400000	2.75700000	14.34710000
N	4.67900000	2.56680000	12.75980000
N	5.32230000	0.79170000	10.51520000
N	3.52920000	3.12070000	9.82280000
N	4.65840000	4.85860000	10.58750000
N	2.67940000	5.30440000	9.31900000
N	6.85170000	3.28450000	9.32190000
N	7.30370000	3.37240000	11.49720000
N	8.97280000	4.17820000	9.98140000
C	2.72460000	4.10560000	14.30410000
H	3.16830000	5.05280000	13.96260000
H	2.25770000	4.28060000	15.28440000
H	1.93040000	3.83660000	13.59150000
C	3.26570000	1.14030000	14.92960000
H	2.51570000	0.79140000	14.20430000
H	2.76980000	1.24910000	15.90530000
H	4.02510000	0.35050000	15.02630000
C	5.39720000	3.25760000	15.56290000
H	6.18200000	2.48880000	15.61680000
H	5.00020000	3.40370000	16.57830000

H	5.87300000	4.19770000	15.24760000
C	4.95440000	-0.33470000	11.34970000
H	3.98900000	-0.77280000	11.02430000
H	4.85980000	-0.02330000	12.39580000
H	5.71040000	-1.13960000	11.28380000
C	5.41580000	0.37670000	9.13040000
H	6.18840000	-0.40350000	8.99820000
H	5.67370000	1.22390000	8.48260000
H	4.45470000	-0.05140000	8.78040000
C	3.59560000	4.46150000	9.89920000
C	1.95020000	4.92740000	8.12970000
H	2.46490000	4.10320000	7.62400000
H	1.91930000	5.78430000	7.43900000
H	0.91170000	4.62280000	8.34410000
C	2.30720000	6.56350000	9.92440000
H	2.74900000	6.64380000	10.92280000
H	1.21170000	6.61070000	10.03450000
H	2.62680000	7.42930000	9.32100000
C	7.74090000	3.61460000	10.24120000
C	9.74500000	3.80950000	8.81760000
H	9.29360000	2.93760000	8.33340000
H	10.76780000	3.53590000	9.12440000
H	9.81910000	4.62770000	8.08130000
C	9.58430000	5.14200000	10.86740000
H	8.84400000	5.52560000	11.57780000
H	9.95690000	5.99440000	10.27670000
H	10.43460000	4.72300000	11.43230000
C	2.27720000	2.39690000	9.78480000
H	1.46380000	2.94410000	10.29160000
H	1.94200000	2.16230000	8.76050000
H	2.41230000	1.43890000	10.30820000
C	6.80800000	3.92040000	8.03110000
H	7.20590000	3.28090000	7.22370000
H	5.75720000	4.13390000	7.77230000
H	7.35890000	4.87730000	7.99990000
C	8.18680000	3.09730000	12.60860000
H	9.14400000	2.66670000	12.27140000
H	8.41040000	3.98990000	13.21650000
H	7.70470000	2.36950000	13.27480000
C	5.30960000	6.12460000	10.37600000
H	4.99810000	6.60320000	9.43210000
H	5.12630000	6.83810000	11.19660000
H	6.39890000	5.96910000	10.32290000

Nugent monomer

HF energy = -672.949627013

No imaginary frequency

Zero-point correction = 0.370563 (Hartree/Particle)

Thermal correction to Energy = 0.393404
Thermal correction to Enthalpy = 0.394348
Thermal correction to Gibbs Free Energy = 0.319140
Sum of electronic and zero-point Energies = -672.579064
Sum of electronic and thermal Energies = -672.556223
Sum of electronic and thermal Enthalpies = -672.555279
Sum of electronic and thermal Free Energies = -672.630487

Coordinates: **Nugent monomer**

Ta	6.95910000	5.10520000	3.69570000
N	8.12000000	5.64100000	5.26240000
N	5.00160000	5.35180000	4.13430000
N	7.46810000	6.15790000	2.04610000
N	7.23810000	3.37450000	3.35940000
C	4.03020000	4.34270000	4.49470000
H	3.53020000	4.59030000	5.44990000
H	3.23970000	4.24920000	3.72550000
H	4.51400000	3.36450000	4.60870000
C	4.37970000	6.65060000	3.98460000
H	3.55600000	6.62140000	3.24650000
H	3.95860000	7.01660000	4.94050000
H	5.09930000	7.40650000	3.62840000
C	7.77870000	6.78360000	6.08240000
H	7.59560000	6.48910000	7.13320000
H	8.58600000	7.54080000	6.08470000
H	6.86080000	7.27910000	5.72490000
C	9.28020000	4.94860000	5.77850000
H	9.10410000	4.57030000	6.80380000
H	9.53680000	4.09590000	5.13710000
H	10.15960000	5.61830000	5.82240000
C	7.79170000	7.56480000	2.15150000
H	7.70270000	7.92500000	3.19010000
H	8.83140000	7.76590000	1.83080000
H	7.12350000	8.18730000	1.52600000
C	7.66130000	5.67310000	0.69730000
H	7.00980000	6.20920000	-0.01810000
H	8.70600000	5.81790000	0.36160000
H	7.42570000	4.60340000	0.63550000
C	7.38080000	1.22090000	4.45150000
H	8.10340000	1.61550000	5.18070000
H	6.37350000	1.33380000	4.87830000
H	7.57830000	0.14700000	4.31110000
C	8.89640000	1.81110000	2.54740000
H	9.64900000	2.20380000	3.24680000
H	9.12170000	0.75080000	2.35520000
H	8.99140000	2.36360000	1.60130000
C	6.45470000	1.43840000	2.13620000
H	6.52010000	1.97530000	1.17880000

H	6.61460000	0.36630000	1.94410000
H	5.43780000	1.57290000	2.53260000
C	7.48950000	1.97830000	3.12570000

Nugent dimer
HF energy = -1345.94148393
No imaginary frequency
Zero-point correction = 0.749536 (Hartree/Particle)
Thermal correction to Energy = 0.791730
Thermal correction to Enthalpy = 0.792674
Thermal correction to Gibbs Free Energy = 0.682435
Sum of electronic and zero-point Energies = -1345.191948
Sum of electronic and thermal Energies = -1345.149754
Sum of electronic and thermal Enthalpies = -1345.148810
Sum of electronic and thermal Free Energies = -1345.259049

Coordinates: **Nugent dimer**

Ta	-1.58420000	-0.15050000	-0.02920000
Ta	1.58470000	0.15060000	-0.03560000
N	-3.36630000	0.87220000	-0.31970000
N	-1.98270000	-1.11450000	-1.79190000
N	-2.25410000	-0.74910000	1.78150000
N	1.97650000	1.11280000	-1.80090000
N	2.26170000	0.75140000	1.77170000
N	3.36580000	-0.87230000	-0.33230000
N	-0.29110000	1.30190000	0.02750000
N	0.29190000	-1.30190000	0.02830000
C	-3.87290000	1.30250000	-1.60890000
H	-4.86490000	0.85530000	-1.81860000
H	-3.18790000	1.02190000	-2.42070000
H	-4.00750000	2.40020000	-1.64450000
C	-4.29230000	1.31360000	0.70220000
H	-4.42790000	2.41350000	0.67910000
H	-3.94300000	1.04220000	1.70580000
H	-5.29790000	0.87040000	0.55180000
C	-3.27150000	-1.70470000	-2.08770000
H	-3.66880000	-1.35600000	-3.06100000
H	-4.01480000	-1.45680000	-1.31750000
H	-3.19600000	-2.80870000	-2.14730000
C	-1.06430000	-1.38820000	-2.87390000
H	-1.09620000	-2.45870000	-3.15970000
H	-0.02890000	-1.15750000	-2.59020000
H	-1.31750000	-0.80620000	-3.78270000
C	-3.36970000	-1.65810000	1.92950000
H	-3.07380000	-2.56770000	2.48730000
H	-3.76410000	-1.97880000	0.95330000
H	-4.20320000	-1.18610000	2.48460000

C	-1.80220000	-0.27860000	3.07160000
H	-2.62340000	0.22200000	3.62280000
H	-0.98360000	0.44320000	2.96610000
H	-1.44860000	-1.11340000	3.70800000
C	1.05430000	1.38580000	-2.88000000
H	1.08520000	2.45610000	-3.16650000
H	0.01980000	1.15530000	-2.59270000
H	1.30440000	0.80320000	-3.78930000
C	3.26410000	1.70280000	-2.10180000
H	3.65780000	1.35390000	-3.07640000
H	4.01030000	1.45500000	-1.33430000
H	3.18860000	2.80680000	-2.16130000
C	3.37890000	1.65930000	1.91440000
H	3.08580000	2.57040000	2.47130000
H	3.77070000	1.97740000	0.93630000
H	4.21350000	1.18740000	2.46780000
C	1.81410000	0.28300000	3.06410000
H	2.63640000	-0.21860000	3.61260000
H	0.99360000	-0.43720000	2.96250000
H	1.46460000	1.11920000	3.70100000
C	4.29560000	-1.31270000	0.68660000
H	4.43110000	-2.41270000	0.66390000
H	3.94990000	-1.04050000	1.69120000
H	5.30060000	-0.86960000	0.53210000
C	3.86740000	-1.30410000	-1.62290000
H	4.85830000	-0.85690000	-1.83730000
H	3.17890000	-1.02480000	-2.43230000
H	4.00220000	-2.40180000	-1.65760000
C	-0.69840000	2.99630000	1.74040000
H	-1.65560000	2.52320000	2.01000000
H	-0.77410000	4.07200000	1.96520000
H	0.09530000	2.56710000	2.37270000
C	0.92560000	3.49400000	-0.06370000
H	1.77480000	3.10110000	0.51240000
H	0.81900000	4.55750000	0.19910000
H	1.17010000	3.43170000	-1.13130000
C	-1.47330000	3.41250000	-0.59150000
H	-1.33390000	3.16850000	-1.65570000
H	-1.43470000	4.50710000	-0.48320000
H	-2.46820000	3.07200000	-0.28690000
C	-0.92520000	-3.49400000	-0.05580000
H	-1.77180000	-3.10070000	0.52370000
H	-0.81740000	-4.55730000	0.20740000
H	-1.17420000	-3.43260000	-1.12240000
C	1.47160000	-3.41330000	-0.59340000
H	1.32790000	-3.17060000	-1.65740000
H	1.43330000	-4.50770000	-0.48370000
H	2.46770000	-3.07250000	-0.29340000

C	0.70600000	-2.99470000	1.74110000
H	1.66430000	-2.52140000	2.00670000
H	0.78260000	-4.07020000	1.96660000
H	-0.08530000	-2.56490000	2.37620000
C	-0.38240000	2.76300000	0.26040000
C	0.38420000	-2.76270000	0.26220000

2) B3LYP geometries and energies for all optimized minima and transition structures (S32-S61)

Species A1

HF energy = -1468.74214362
No imaginary frequency
Zero-point correction = 0.561032 (Hartree/Particle)
Thermal correction to Energy = 0.597566
Thermal correction to Enthalpy = 0.598510
Thermal correction to Gibbs Free Energy = 0.497075
Sum of electronic and zero-point Energies = -1468.181111
Sum of electronic and thermal Energies = -1468.144578
Sum of electronic and thermal Enthalpies = -1468.143634
Sum of electronic and thermal Free Energies = -1468.245069

Coordinates: **A1**

Ta	7.09400000	5.23350000	3.57650000
N	6.24580000	6.85540000	2.63560000
N	8.06530000	5.93040000	5.19980000
N	5.22270000	4.96840000	4.46770000
N	8.66970000	5.47240000	2.23300000
N	7.20920000	3.12500000	3.41100000
C	6.92400000	8.14500000	2.55290000
H	6.99920000	8.50830000	1.51190000
H	6.37020000	8.91280000	3.12330000
H	7.93810000	8.08730000	2.95860000
C	4.93250000	6.94240000	2.01680000
H	4.35180000	7.78700000	2.42870000
H	5.00770000	7.10610000	0.92580000
H	4.36200000	6.02430000	2.18010000
C	4.31190000	3.83240000	4.46340000
H	3.94000000	3.61430000	5.48020000
H	3.42180000	4.03340000	3.83700000
H	4.81180000	2.94220000	4.08350000
C	4.52900000	6.10970000	5.06700000
H	3.58060000	6.33360000	4.54790000
H	4.27430000	5.89540000	6.12010000
H	5.14970000	7.01020000	5.04330000
C	7.58970000	5.80250000	6.58020000
H	8.34380000	5.29700000	7.20680000
H	7.40640000	6.79660000	7.02280000
H	6.66420000	5.22660000	6.62210000
C	9.27990000	6.74870000	5.17980000
H	10.07600000	6.28220000	5.78520000
H	9.64960000	6.87900000	4.16160000
H	9.08210000	7.74520000	5.61050000
C	8.69800000	6.06290000	0.90330000
H	7.73280000	6.50870000	0.65520000

H	9.47560000	6.84480000	0.82310000
H	8.93260000	5.30490000	0.13360000
C	9.94980000	4.81340000	2.48530000
H	10.12850000	3.97960000	1.78530000
H	10.78580000	5.52630000	2.36440000
H	10.00050000	4.41310000	3.50010000
Si	6.75550000	2.42440000	1.85160000
Si	7.79480000	2.09460000	4.73160000
C	6.57310000	1.98110000	6.18130000
H	6.30370000	2.96360000	6.58640000
H	5.64250000	1.47840000	5.88930000
H	7.02330000	1.39490000	6.99520000
C	9.45340000	2.67840000	5.45460000
H	9.44880000	3.73100000	5.75790000
H	9.68480000	2.07430000	6.34390000
H	10.27570000	2.53340000	4.74120000
C	8.12910000	0.29280000	4.21650000
H	8.73180000	0.19530000	3.30520000
H	8.69800000	-0.17990000	5.03010000
H	7.21280000	-0.29250000	4.08200000
C	5.63830000	0.88770000	1.98160000
H	4.85540000	0.99430000	2.74380000
H	5.13180000	0.74250000	1.01630000
H	6.19200000	-0.03250000	2.19600000
C	8.24130000	1.94600000	0.76950000
H	8.97440000	1.33010000	1.30510000
H	7.89910000	1.36960000	-0.10220000
H	8.76430000	2.83410000	0.39340000
C	5.72190000	3.66070000	0.84190000
H	4.73470000	3.83390000	1.28990000
H	6.20040000	4.63390000	0.67870000
H	5.55080000	3.22190000	-0.15220000

Species A2

HF energy = -1468.73411441

no imaginary frequency

Zero-point correction = 0.562411 (Hartree/Particle)
Thermal correction to Energy = 0.598383
Thermal correction to Enthalpy = 0.599327
Thermal correction to Gibbs Free Energy = 0.498150
Sum of electronic and zero-point Energies = -1468.171704
Sum of electronic and thermal Energies = -1468.135732
Sum of electronic and thermal Enthalpies = -1468.134787
Sum of electronic and thermal Free Energies = -1468.235965

Coordinates: **A2**

Ta	7.05080000	5.21620000	3.60200000
N	5.86580000	6.01580000	2.06810000

N	8.09020000	5.81800000	5.32080000
N	5.33070000	5.40050000	4.73060000
N	8.66890000	6.02690000	2.60660000
N	7.25450000	3.20760000	3.33220000
C	4.40700000	5.90900000	1.98110000
H	3.91830000	6.89650000	2.06750000
H	4.10990000	5.50190000	0.99820000
H	4.00550000	5.25430000	2.75530000
C	6.28660000	6.85780000	0.94920000
H	5.90630000	6.45790000	-0.00740000
H	5.88280000	7.88320000	1.04330000
H	7.37000000	6.92020000	0.87960000
C	4.75020000	4.32550000	5.52680000
H	4.84710000	4.50550000	6.61440000
H	3.66960000	4.22700000	5.31430000
H	5.22270000	3.36670000	5.29780000
C	4.61050000	6.64540000	4.95900000
H	3.54100000	6.54350000	4.70450000
H	4.65810000	6.96200000	6.01620000
H	5.02850000	7.45300000	4.34750000
C	7.54200000	6.24450000	6.60690000
H	8.00560000	5.68250000	7.43700000
H	7.74900000	7.31430000	6.79760000
H	6.46680000	6.08940000	6.65530000
C	9.54320000	5.98210000	5.41200000
H	9.93930000	5.42330000	6.27830000
H	10.04350000	5.61720000	4.51420000
H	9.82760000	7.03830000	5.56900000
C	9.11000000	7.40990000	2.72380000
H	8.55100000	7.93040000	3.50940000
H	10.18390000	7.46940000	2.97310000
H	8.96990000	7.96910000	1.78140000
C	9.44570000	5.33400000	1.58520000
H	9.29550000	5.76420000	0.57660000
H	10.52670000	5.40790000	1.80580000
H	9.18660000	4.27280000	1.54320000
Si	6.61220000	2.35450000	1.87600000
Si	8.07410000	2.13570000	4.53150000
C	8.12670000	2.78680000	6.30660000
H	8.86130000	3.58230000	6.44890000
H	7.15940000	3.15240000	6.66770000
H	8.41800000	1.94030000	6.94670000
C	9.87390000	1.84080000	4.01600000
H	10.41380000	2.79580000	3.95850000
H	10.38390000	1.22090000	4.76700000
H	9.97710000	1.34220000	3.04600000
C	7.15360000	0.48140000	4.73980000
H	6.98740000	-0.10840000	3.83400000

H	7.73900000	-0.14170000	5.43150000
H	6.17620000	0.64830000	5.21370000
C	4.89130000	1.65810000	2.25340000
H	4.20770000	2.47360000	2.52680000
H	4.47580000	1.16410000	1.36370000
H	4.88640000	0.93090000	3.07300000
C	7.78990000	0.97660000	1.29650000
H	8.07260000	0.22680000	2.03980000
H	7.30380000	0.44600000	0.46500000
H	8.71550000	1.41340000	0.89640000
C	6.44580000	3.41210000	0.31680000
H	5.58050000	4.07770000	0.33930000
H	7.33330000	4.01970000	0.10910000
H	6.31700000	2.71890000	-0.52800000

Species A3
HF energy = -1468.72932847
No imaginary frequency
Zero-point correction = 0.560701 (Hartree/Particle)
Thermal correction to Energy = 0.597496
Thermal correction to Enthalpy = 0.598440
Thermal correction to Gibbs Free Energy = 0.495754
Sum of electronic and zero-point Energies = -1468.168627
Sum of electronic and thermal Energies = -1468.131833
Sum of electronic and thermal Enthalpies = -1468.130888
Sum of electronic and thermal Free Energies = -1468.233575

Coordinates: **A3**

Ta	7.11080000	5.14830000	3.55870000
N	7.05060000	7.26210000	3.58150000
N	7.39150000	5.13320000	5.56970000
N	5.15560000	5.19960000	3.07450000
N	8.66220000	5.40320000	2.27370000
N	7.23820000	2.99150000	3.36280000
C	8.05380000	8.23510000	3.17320000
H	7.68430000	8.90520000	2.37220000
H	8.33790000	8.88990000	4.01750000
H	8.95940000	7.74110000	2.81790000
C	5.97240000	7.98390000	4.25540000
H	6.34940000	8.53440000	5.13590000
H	5.50500000	8.73540000	3.59120000
H	5.18780000	7.30140000	4.59480000
C	4.21670000	4.18490000	3.55470000
H	3.39910000	4.65650000	4.12690000
H	3.76110000	3.63600000	2.71280000
H	4.71520000	3.45350000	4.19440000
C	4.48040000	6.13290000	2.17810000
H	4.07400000	5.60660000	1.29890000

H	3.63510000	6.62600000	2.68710000
H	5.17310000	6.90360000	1.83320000
C	6.31120000	5.12580000	6.54710000
H	6.60470000	4.57430000	7.45640000
H	6.04050000	6.15130000	6.85700000
H	5.41150000	4.64960000	6.14380000
C	8.56110000	5.82620000	6.09680000
H	8.92940000	5.33660000	7.01420000
H	9.38590000	5.82780000	5.37340000
H	8.33130000	6.87910000	6.33790000
C	8.64780000	6.02890000	0.96220000
H	7.68340000	6.51280000	0.77180000
H	9.43160000	6.80090000	0.86870000
H	8.82400000	5.28660000	0.16420000
C	9.97510000	4.86860000	2.60770000
H	10.30600000	4.11790000	1.87020000
H	10.73560000	5.66980000	2.63980000
H	9.96780000	4.37370000	3.58500000
Si	6.98050000	2.29630000	1.75270000
Si	7.72450000	1.87710000	4.65330000
C	6.38140000	1.65040000	5.97970000
H	6.19400000	2.53930000	6.58790000
H	5.43010000	1.34900000	5.51840000
H	6.67710000	0.84140000	6.66330000
C	9.36480000	2.34760000	5.49100000
H	9.36650000	3.34770000	5.93230000
H	9.57450000	1.62920000	6.29670000
H	10.19960000	2.28120000	4.77890000
C	8.05640000	0.07880000	4.09680000
H	8.68840000	-0.02550000	3.20760000
H	8.58690000	-0.41500000	4.92430000
H	7.13610000	-0.49030000	3.92490000
C	5.81490000	0.78550000	1.75320000
H	4.99530000	0.90410000	2.47490000
H	5.35890000	0.69060000	0.75720000
H	6.31700000	-0.16230000	1.97110000
C	8.60510000	1.80670000	0.88790000
H	9.29360000	1.24250000	1.52770000
H	8.38980000	1.18780000	0.00480000
H	9.13770000	2.70070000	0.53780000
C	6.12300000	3.46160000	0.51540000
H	5.06260000	3.60440000	0.75220000
H	6.58030000	4.44910000	0.39910000
H	6.16870000	2.96940000	-0.46810000

Species TSA2BC
HF energy = -1468.69719710
Imaginary frequency: 112*i*

Zero-point correction = 0.562083 (Hartree/Particle)
Thermal correction to Energy = 0.597291
Thermal correction to Enthalpy = 0.598235
Thermal correction to Gibbs Free Energy = 0.500271
Sum of electronic and zero-point Energies = -1468.135115
Sum of electronic and thermal Energies = -1468.099906
Sum of electronic and thermal Enthalpies = -1468.098962
Sum of electronic and thermal Free Energies = -1468.196927

Coordinates: **TSA2BC**

Ta	8.10290000	5.48420000	4.34200000
N	7.37440000	6.06740000	6.13650000
N	6.17030000	5.08280000	3.67770000
N	8.38760000	6.73190000	2.77400000
N	8.97590000	3.73090000	4.35240000
C	5.15880000	4.47740000	4.54220000
H	4.32630000	5.17960000	4.73310000
H	4.71650000	3.57980000	4.07700000
H	5.58380000	4.18030000	5.50560000
C	5.55580000	5.39890000	2.39480000
H	5.15270000	4.49560000	1.90240000
H	4.70370000	6.09340000	2.52100000
H	6.27680000	5.86050000	1.71620000
C	6.40480000	7.15480000	6.23980000
H	5.48800000	6.81560000	6.75100000
H	6.81360000	8.00320000	6.81490000
H	6.10960000	7.52040000	5.25040000
C	7.59110000	5.45530000	7.44200000
H	6.64350000	5.05460000	7.84310000
H	8.30450000	4.63130000	7.38580000
H	7.97290000	6.18740000	8.17450000
C	7.82840000	8.07930000	2.74660000
H	7.34950000	8.33370000	3.69930000
H	8.61770000	8.82810000	2.56660000
H	7.07310000	8.19000000	1.94880000
C	9.05010000	6.41770000	1.51210000
H	8.33770000	6.46890000	0.66970000
H	9.86460000	7.12960000	1.30020000
H	9.47490000	5.41060000	1.53090000
Si	8.52840000	2.29510000	3.39260000
C	7.08430000	1.32460000	4.14790000
H	7.28190000	1.01860000	5.18180000
H	6.16080000	1.91480000	4.14500000
H	6.89770000	0.41450000	3.55990000
C	9.97020000	1.08940000	3.10870000
H	10.45320000	0.72070000	4.01870000
H	9.57500000	0.21820000	2.56570000
H	10.74810000	1.53630000	2.47680000

C	8.02330000	2.78200000	1.62710000
H	8.85980000	3.22760000	1.07180000
H	7.72520000	1.87460000	1.08160000
H	7.18050000	3.47920000	1.59330000
Si	10.44790000	3.73140000	5.66300000
N	10.23230000	5.85940000	5.07000000
C	11.18630000	6.11810000	3.97900000
H	11.11280000	5.35020000	3.20430000
H	10.99580000	7.09830000	3.51160000
H	12.22400000	6.12400000	4.35070000
C	10.40470000	6.95600000	6.03610000
H	10.07720000	7.91730000	5.59960000
H	9.82400000	6.78470000	6.94360000
H	11.46020000	7.08070000	6.32460000
C	11.18690000	4.38350000	7.34060000
H	10.45470000	4.73960000	8.07730000
H	11.70740000	3.53540000	7.80690000
H	11.92420000	5.18180000	7.19840000
C	9.75130000	2.11940000	6.51400000
H	9.42600000	1.31640000	5.84560000
H	10.51240000	1.69520000	7.18450000
H	8.88390000	2.36510000	7.14720000
C	12.02530000	3.24340000	4.70400000
H	12.36520000	2.26660000	5.07390000
H	11.89280000	3.15400000	3.62150000
H	12.83600000	3.95880000	4.88690000

Species B

HF energy = -924.912256214
No imaginary frequency
Zero-point correction = 0.361801 (Hartree/Particle)
Thermal correction to Energy = 0.387541
Thermal correction to Enthalpy = 0.388486
Thermal correction to Gibbs Free Energy = 0.304578
Sum of electronic and zero-point Energies = -924.550456
Sum of electronic and thermal Energies = -924.524715
Sum of electronic and thermal Enthalpies = -924.523771
Sum of electronic and thermal Free Energies = -924.607678

Coordinates: **B**

Ta	6.94520000	5.21780000	3.72410000
N	7.98000000	5.75400000	5.38410000
N	4.96120000	5.51710000	4.01980000
N	7.57380000	6.31200000	2.13630000
N	7.23560000	3.46470000	3.38850000
C	3.94660000	4.50140000	4.27620000
H	3.41240000	4.70190000	5.22180000
H	3.19230000	4.47670000	3.46950000

H	4.40700000	3.51180000	4.34450000
C	4.36690000	6.84320000	3.89710000
H	3.62690000	6.87960000	3.07800000
H	3.85180000	7.14340000	4.82670000
H	5.12910000	7.60390000	3.67930000
C	7.63760000	6.95290000	6.14050000
H	7.32320000	6.70430000	7.16970000
H	8.49480000	7.64560000	6.21070000
H	6.80700000	7.49810000	5.67150000
C	9.05830000	5.01060000	6.02530000
H	8.78520000	4.71730000	7.05480000
H	9.28350000	4.10240000	5.45940000
H	9.97860000	5.61790000	6.08780000
C	7.86050000	7.73660000	2.25790000
H	7.65460000	8.10060000	3.27390000
H	8.92170000	7.95460000	2.04300000
H	7.24840000	8.33350000	1.55880000
C	7.87650000	5.82130000	0.79660000
H	7.26450000	6.33760000	0.03600000
H	8.93700000	5.99130000	0.53800000
H	7.67530000	4.74850000	0.72900000
Si	7.53040000	1.78150000	3.08250000
C	8.12550000	0.93630000	4.67150000
H	9.06510000	1.37960000	5.02820000
H	7.38440000	1.04090000	5.47540000
H	8.30240000	-0.13730000	4.51690000
C	8.86100000	1.59350000	1.74560000
H	9.79750000	2.08000000	2.05020000
H	9.08350000	0.53630000	1.54430000
H	8.54250000	2.05170000	0.79950000
C	5.93520000	0.94520000	2.49210000
H	5.55760000	1.41930000	1.57610000
H	6.09470000	-0.12060000	2.27580000
H	5.14440000	1.01500000	3.25130000

Species C

HF energy = -543.848019144
No imaginary frequency
Zero-point correction = 0.194179 (Hartree/Particle)
Thermal correction to Energy = 0.206147
Thermal correction to Enthalpy = 0.207091
Thermal correction to Gibbs Free Energy = 0.157219
Sum of electronic and zero-point Energies = -543.653840
Sum of electronic and thermal Energies = -543.641872
Sum of electronic and thermal Enthalpies = -543.640928
Sum of electronic and thermal Free Energies = -543.690801

Coordinates: **C**

Si	-0.83510000	0.87850000	0.11010000
N	-0.16780000	1.82620000	-1.20630000
C	1.21650000	1.68340000	-1.63230000
H	1.58410000	0.67130000	-1.43070000
H	1.30380000	1.85680000	-2.71760000
H	1.89800000	2.39850000	-1.13310000
C	-0.70590000	3.13700000	-1.54050000
H	-0.63050000	3.31880000	-2.62540000
H	-1.76560000	3.20560000	-1.27000000
H	-0.17230000	3.96360000	-1.03350000
C	-0.38850000	1.56020000	1.82680000
H	-0.75380000	2.58760000	1.96230000
H	-0.82640000	0.94870000	2.62860000
H	0.69890000	1.57680000	1.98340000
C	-2.72030000	0.85670000	-0.05300000
H	-3.03100000	0.49290000	-1.04090000
H	-3.15410000	0.18570000	0.70130000
H	-3.17540000	1.84400000	0.09880000
C	-0.17380000	-0.88920000	-0.02500000
H	-0.68010000	-1.53280000	0.70750000
H	-0.35620000	-1.31340000	-1.02090000
H	0.90260000	-0.95860000	0.17830000

Species D

HF energy = -1849.82190022
No imaginary frequency
Zero-point correction = 0.730030 (Hartree/Particle)
Thermal correction to Energy = 0.779494
Thermal correction to Enthalpy = 0.780438
Thermal correction to Gibbs Free Energy = 0.651068
Sum of electronic and zero-point Energies = -1849.091870
Sum of electronic and thermal Energies = -1849.042406
Sum of electronic and thermal Enthalpies = -1849.041462
Sum of electronic and thermal Free Energies = -1849.170832

Coordinates: **D**

Ta	26.14730000	15.93240000	14.60540000
Ta	25.32680000	13.69520000	12.41980000
N	26.48440000	17.98620000	14.76590000
N	24.41050000	16.24830000	15.65510000
N	27.90160000	15.56710000	15.53560000
N	23.82540000	14.58880000	11.33860000
N	26.89010000	12.80780000	11.50520000
N	24.22840000	11.92530000	12.27210000
N	26.19370000	15.70860000	12.64350000
N	25.49050000	13.84590000	14.38270000
Si	26.87040000	16.70670000	11.36280000
Si	25.32500000	12.65750000	15.66950000

C	25.45000000	19.01650000	14.72370000
H	25.43960000	19.61100000	15.65610000
H	24.46030000	18.57230000	14.58820000
H	25.61970000	19.72650000	13.89770000
C	27.78230000	18.64230000	14.88860000
H	27.98040000	19.31170000	14.03190000
H	28.59220000	17.91010000	14.93670000
H	27.82830000	19.27170000	15.79770000
C	24.33680000	17.04260000	16.87750000
H	23.58440000	17.84680000	16.79550000
H	25.29980000	17.50790000	17.10630000
H	24.04530000	16.41250000	17.73650000
C	23.09290000	15.70540000	15.34990000
H	22.70350000	15.11300000	16.19750000
H	23.12390000	15.05250000	14.47560000
H	22.36350000	16.51270000	15.15640000
C	28.19730000	15.96410000	16.90730000
H	28.48590000	15.09280000	17.51880000
H	27.32940000	16.43360000	17.38200000
H	29.03350000	16.68380000	16.94170000
C	29.05350000	14.92170000	14.91720000
H	29.95070000	15.56120000	14.99500000
H	28.87120000	14.73230000	13.85720000
H	29.28730000	13.96180000	15.41020000
C	23.19780000	15.87590000	11.60910000
H	23.30600000	16.55760000	10.74610000
H	23.65020000	16.36210000	12.47500000
H	22.11510000	15.76090000	11.79760000
C	23.24930000	14.01390000	10.12660000
H	22.15200000	13.91680000	10.20420000
H	23.65910000	13.01990000	9.92570000
H	23.45650000	14.65620000	9.25220000
C	26.85110000	12.33770000	10.12500000
H	27.66570000	12.78510000	9.53120000
H	25.90370000	12.59980000	9.64240000
H	26.96730000	11.24120000	10.07430000
C	28.16870000	12.49210000	12.13080000
H	28.39590000	11.41520000	12.03850000
H	28.15410000	12.73870000	13.19460000
H	28.99550000	13.04650000	11.65320000
C	24.77280000	10.57630000	12.15630000
H	24.48360000	9.94700000	13.01740000
H	25.86440000	10.59420000	12.10630000
H	24.39130000	10.06670000	11.25110000
C	22.77110000	11.83360000	12.31180000
H	22.37250000	11.40170000	11.37500000
H	22.32000000	12.81920000	12.45570000
H	22.42830000	11.18100000	13.13110000

C	28.75620000	16.83750000	11.56180000
H	29.03740000	17.28610000	12.52340000
H	29.18920000	17.46030000	10.76580000
H	29.23180000	15.84890000	11.50120000
C	26.57090000	15.97190000	9.63730000
H	27.05090000	14.99460000	9.51180000
H	26.99750000	16.64700000	8.88130000
H	25.50330000	15.85570000	9.41390000
C	26.16960000	18.46840000	11.29240000
H	25.07380000	18.48110000	11.35010000
H	26.45650000	18.93750000	10.34040000
H	26.55660000	19.09660000	12.10110000
C	25.56040000	13.41450000	17.39530000
H	26.55020000	13.86610000	17.52700000
H	25.45840000	12.62100000	18.15000000
H	24.80740000	14.18070000	17.61710000
C	23.63430000	11.80010000	15.72280000
H	22.80450000	12.51310000	15.63690000
H	23.52100000	11.27300000	16.68110000
H	23.52600000	11.06090000	14.92310000
C	26.65640000	11.31310000	15.49020000
H	26.60040000	10.81240000	14.51510000
H	26.54220000	10.54300000	16.26660000
H	27.66550000	11.73590000	15.59190000

Species E

HF energy = -227.391731019
No imaginary frequency
Zero-point correction = 0.090470 (Hartree/Particle)
Thermal correction to Energy = 0.097051
Thermal correction to Enthalpy = 0.097995
Thermal correction to Gibbs Free Energy = 0.060191
Sum of electronic and zero-point Energies = -227.301261
Sum of electronic and thermal Energies = -227.294680
Sum of electronic and thermal Enthalpies = -227.293736
Sum of electronic and thermal Free Energies = -227.331540

Coordinates: **E**

C	-0.92550000	0.21710000	-0.41760000
N	0.18090000	-0.15490000	-0.79150000
N	-2.09600000	0.48500000	-0.17200000
C	1.27880000	-0.58710000	0.06160000
H	1.56600000	-1.60900000	-0.21510000
H	2.14850000	0.05860000	-0.11280000
H	1.03380000	-0.56880000	1.13240000
C	-2.64280000	1.81120000	0.07760000
H	-3.43890000	2.01260000	-0.64970000
H	-3.09560000	1.83390000	1.07670000

H	-1.89430000	2.61260000	0.01030000

Species TSBEF
HF energy = -1152.29269166
Imaginary frequency: 209*i*
Zero-point correction = 0.452730 (Hartree/Particle)
Thermal correction to Energy = 0.485611
Thermal correction to Enthalpy = 0.486555
Thermal correction to Gibbs Free Energy = 0.385367
Sum of electronic and zero-point Energies = -1151.839962
Sum of electronic and thermal Energies = -1151.807081
Sum of electronic and thermal Enthalpies = -1151.806137
Sum of electronic and thermal Free Energies = -1151.907324

Coordinates: **TSBEF**

Ta	6.45350000	5.19800000	4.18880000
N	7.57470000	6.22650000	5.69770000
N	4.54580000	5.48260000	3.47440000
N	7.38510000	6.07540000	2.59470000
N	7.04850000	3.48900000	4.06760000
C	4.06600000	4.81140000	2.27420000
H	3.14040000	4.23910000	2.47170000
H	3.83870000	5.53440000	1.46860000
H	4.81900000	4.11360000	1.89250000
C	3.55870000	6.41290000	3.99340000
H	3.33200000	7.21580000	3.26690000
H	2.59840000	5.91310000	4.22400000
H	3.91140000	6.88890000	4.91730000
C	7.56820000	7.68200000	5.61310000
H	7.73950000	8.14060000	6.60270000
H	8.34230000	8.06500000	4.92350000
H	6.59470000	8.05080000	5.25630000
C	8.87740000	5.73480000	6.13760000
H	9.17240000	6.19710000	7.09590000
H	8.84810000	4.64800000	6.27000000
H	9.67620000	5.96580000	5.40820000
C	6.92100000	7.31550000	1.98620000
H	5.95730000	7.62270000	2.40940000
H	7.63900000	8.14310000	2.13140000
H	6.78270000	7.19440000	0.89620000
C	8.61190000	5.61770000	1.95490000
H	8.46340000	5.47750000	0.86810000
H	9.43290000	6.34840000	2.07610000
H	8.93290000	4.66460000	2.38260000
Si	7.40370000	1.81060000	3.83540000
C	8.34840000	1.14570000	5.34080000
H	9.28980000	1.69270000	5.48730000
H	7.75550000	1.25450000	6.25940000

H	8.59600000	0.08070000	5.22860000
C	8.47270000	1.56600000	2.28780000
H	9.43660000	2.08420000	2.38140000
H	8.68460000	0.50180000	2.11230000
H	7.97090000	1.95860000	1.39330000
C	5.80030000	0.81620000	3.63260000
H	5.23060000	1.16320000	2.75990000
H	5.99980000	-0.25620000	3.49730000
H	5.15320000	0.92690000	4.51350000
C	5.93220000	5.64440000	7.17580000
N	5.35440000	5.00730000	6.23820000
N	6.02360000	6.21220000	8.25220000
C	4.22790000	4.12230000	6.58710000
H	3.47030000	4.21050000	5.80340000
H	4.57440000	3.08160000	6.61300000
H	3.78910000	4.38550000	7.55700000
C	7.03550000	6.16820000	9.28760000
H	7.67740000	7.05510000	9.22130000
H	6.54020000	6.18940000	10.26490000
H	7.66470000	5.27080000	9.22740000

Species F

HF energy = -1152.33754588
No imaginary frequency
Zero-point correction= 0.458745 (Hartree/Particle)
Thermal correction to Energy= 0.489825
Thermal correction to Enthalpy= 0.490769
Thermal correction to Gibbs Free Energy= 0.396798
Sum of electronic and zero-point Energies= -1151.878801
Sum of electronic and thermal Energies= -1151.847721
Sum of electronic and thermal Enthalpies= -1151.846777
Sum of electronic and thermal Free Energies= -1151.940748

Coordinates: **F**

Ta	6.24090000	5.18940000	4.01000000
N	7.41160000	5.73230000	6.15370000
N	4.56450000	5.09440000	2.88010000
N	7.40430000	6.57000000	3.06020000
N	6.98490000	3.54980000	3.80090000
C	4.01650000	3.95190000	2.16100000
H	2.99980000	3.70460000	2.51600000
H	3.94210000	4.16320000	1.07900000
H	4.65520000	3.07700000	2.29770000
C	3.74570000	6.28320000	2.66950000
H	3.72960000	6.57860000	1.60580000
H	2.70070000	6.11420000	2.98440000
H	4.12250000	7.13730000	3.24720000
C	8.06050000	7.06070000	6.17800000

H	8.49220000	7.29270000	7.16110000
H	8.85550000	7.07820000	5.42520000
H	7.32650000	7.83190000	5.92720000
C	8.33940000	4.68030000	6.62100000
H	8.75570000	4.90440000	7.61230000
H	7.81180000	3.72450000	6.65830000
H	9.16050000	4.59400000	5.90140000
C	7.04250000	7.98000000	3.02030000
H	6.16040000	8.18610000	3.64300000
H	7.86090000	8.62200000	3.39500000
H	6.80720000	8.31260000	1.99350000
C	8.59680000	6.30910000	2.26420000
H	8.44420000	6.59020000	1.20620000
H	9.46290000	6.89150000	2.63160000
H	8.85510000	5.24720000	2.30090000
Si	7.57080000	1.91580000	3.74640000
C	9.46720000	1.91180000	3.80660000
H	9.89090000	2.48560000	2.97120000
H	9.84320000	2.35450000	4.73880000
H	9.86580000	0.88950000	3.74310000
C	7.01750000	1.08660000	2.13400000
H	7.34820000	1.66240000	1.25930000
H	7.43360000	0.07310000	2.04570000
H	5.92420000	0.99940000	2.08000000
C	6.90200000	0.91090000	5.20950000
H	5.80350000	0.91080000	5.21550000
H	7.23580000	-0.13550000	5.16720000
H	7.23470000	1.32470000	6.17120000
C	6.08440000	5.70690000	6.83170000
N	5.17660000	5.54230000	5.82220000
N	5.78950000	5.79490000	8.07000000
C	3.77630000	5.42360000	6.20550000
H	3.17540000	5.24810000	5.30910000
H	3.62950000	4.59050000	6.90760000
H	3.42590000	6.33580000	6.70930000
C	6.75180000	5.96070000	9.13780000
H	7.70850000	6.42750000	8.85870000
H	6.30350000	6.58420000	9.92270000
H	6.98150000	4.98930000	9.60390000

Species TSFG1
HF energy = -1152.31334403
Imaginary frequency: 77*i*
Zero-point correction= 0.456881 (Hartree/Particle)
Thermal correction to Energy= 0.488118
Thermal correction to Enthalpy= 0.489063
Thermal correction to Gibbs Free Energy= 0.392688
Sum of electronic and zero-point Energies= -1151.856463

Sum of electronic and thermal Energies= -1151.825226
Sum of electronic and thermal Enthalpies= -1151.824281
Sum of electronic and thermal Free Energies= -1151.920656

Coordinates: **TSFG1**

Ta	6.11180000	5.31080000	3.79570000
N	7.58940000	5.56360000	7.40100000
N	4.16780000	4.92740000	3.43080000
N	6.75730000	6.37000000	2.20280000
N	7.06740000	3.76990000	3.84040000
C	3.54550000	3.67540000	3.02440000
H	2.91340000	3.26260000	3.83070000
H	2.90130000	3.82150000	2.13960000
H	4.31110000	2.93530000	2.77410000
C	3.18020000	5.93500000	3.79940000
H	2.52810000	6.18900000	2.94530000
H	2.54200000	5.58890000	4.62950000
H	3.66430000	6.86370000	4.13660000
C	8.78440000	6.37150000	7.17990000
H	9.37160000	6.37800000	8.10770000
H	9.41290000	5.96820000	6.37010000
H	8.52540000	7.40240000	6.93660000
C	7.89840000	4.27260000	8.01250000
H	8.09380000	4.37600000	9.08940000
H	7.08560000	3.56350000	7.86780000
H	8.79790000	3.84500000	7.54100000
C	5.89330000	7.20700000	1.37830000
H	4.88070000	7.26230000	1.79420000
H	6.28770000	8.23570000	1.30450000
H	5.81000000	6.80900000	0.35110000
C	8.10390000	6.28740000	1.64750000
H	8.09090000	5.86770000	0.62550000
H	8.56920000	7.28690000	1.59100000
H	8.73820000	5.65120000	2.27160000
Si	8.00970000	2.31920000	3.77870000
C	9.83870000	2.70380000	4.10770000
H	10.23800000	3.40440000	3.36160000
H	9.97610000	3.16150000	5.09690000
H	10.45560000	1.79470000	4.07300000
C	7.84860000	1.52270000	2.06530000
H	8.20210000	2.20500000	1.28040000
H	8.43040000	0.59330000	1.98870000
H	6.80070000	1.27960000	1.84250000
C	7.39660000	1.09050000	5.08700000
H	6.33130000	0.86420000	4.94450000
H	7.94970000	0.14170000	5.04150000
H	7.51530000	1.49690000	6.10030000
C	6.48990000	5.72800000	6.56730000

N	6.69070000	6.51070000	5.39250000
N	5.30070000	5.23360000	6.70790000
C	6.27390000	7.91210000	5.49290000
H	6.34560000	8.38050000	4.50330000
H	5.23830000	8.01860000	5.86040000
H	6.92410000	8.49050000	6.16980000
C	4.86320000	4.54120000	7.90710000
H	5.39910000	4.85310000	8.81780000
H	3.79610000	4.75370000	8.05240000
H	4.95340000	3.44760000	7.81290000

Species G1

HF energy = -1152.35101412
No imaginary frequency
Zero-point correction = 0.457190 (Hartree/Particle)
Thermal correction to Energy = 0.489245
Thermal correction to Enthalpy = 0.490190
Thermal correction to Gibbs Free Energy = 0.391762
Sum of electronic and zero-point Energies = -1151.893824
Sum of electronic and thermal Energies = -1151.861769
Sum of electronic and thermal Enthalpies = -1151.860825
Sum of electronic and thermal Free Energies = -1151.959252

Coordinates: **G1**

Ta	5.29170000	3.08970000	11.15340000
Si	4.38240000	3.25170000	14.56540000
N	4.90930000	3.15670000	12.91910000
N	5.67760000	1.12190000	10.73990000
N	3.44290000	2.89460000	9.89220000
N	4.33700000	4.88080000	10.23040000
N	2.26880000	4.80860000	9.00540000
C	3.15890000	4.68610000	14.77570000
H	3.62310000	5.64240000	14.49900000
H	2.80530000	4.77250000	15.81290000
H	2.27890000	4.54690000	14.13280000
C	3.52470000	1.63790000	15.07310000
H	2.64530000	1.44650000	14.44290000
H	3.18650000	1.66920000	16.11850000
H	4.20040000	0.77870000	14.96610000
C	5.87330000	3.54280000	15.70150000
H	6.61110000	2.73560000	15.59930000
H	5.57460000	3.59130000	16.75820000
H	6.37930000	4.48630000	15.45560000
C	6.10810000	0.12930000	11.71480000
H	5.44400000	-0.75550000	11.70840000
H	6.10160000	0.55540000	12.72190000
H	7.13190000	-0.23070000	11.50110000

C	5.63110000	0.55820000	9.40080000
H	6.62880000	0.22290000	9.06110000
H	5.25480000	1.29410000	8.67900000
H	4.96120000	-0.32120000	9.35330000
C	3.30830000	4.21820000	9.68540000
C	1.57520000	4.12550000	7.92390000
H	2.18810000	3.30030000	7.55490000
H	1.41960000	4.83140000	7.09570000
H	0.59270000	3.73400000	8.22900000
C	1.73510000	6.10800000	9.38970000
H	2.18300000	6.43120000	10.33110000
H	0.64820000	6.02790000	9.54080000
H	1.91770000	6.87590000	8.62300000
C	2.30920000	1.98610000	9.98760000
H	1.43470000	2.45870000	10.46240000
H	1.98980000	1.58770000	9.01250000
H	2.60790000	1.13130000	10.60360000
C	4.78710000	6.19010000	9.79400000
H	4.47530000	6.41260000	8.76220000
H	4.41950000	7.00120000	10.44160000
H	5.88180000	6.21440000	9.83470000
N	7.13780000	3.93180000	10.96550000
C	7.90220000	4.68220000	11.94810000
H	8.12060000	5.70920000	11.59830000
H	7.34690000	4.74950000	12.88750000
H	8.87470000	4.19830000	12.15550000
C	7.85860000	3.79510000	9.70960000
H	7.27350000	3.22020000	8.97660000
H	8.08490000	4.77630000	9.25160000
H	8.81890000	3.26540000	9.84720000

Species TSG1G2
HF energy = -1152.34324513
Imaginary frequency: 28*i*
Zero-point correction= 0.457950 (Hartree/Particle)
Thermal correction to Energy= 0.488841
Thermal correction to Enthalpy= 0.489785
Thermal correction to Gibbs Free Energy= 0.395193
Sum of electronic and zero-point Energies= -1151.885296
Sum of electronic and thermal Energies= -1151.854405
Sum of electronic and thermal Enthalpies= -1151.853460
Sum of electronic and thermal Free Energies= -1151.948052

Coordinates: **TSG1G2**

Ta	5.24270000	2.45620000	10.89790000
Si	4.09440000	3.09600000	14.17960000
N	4.54290000	2.64180000	12.56690000
N	5.69800000	0.50140000	10.78870000

N	3.61180000	2.85940000	9.72980000
N	6.63250000	3.34930000	9.20120000
N	7.13670000	3.49260000	11.36120000
N	8.72780000	4.37500000	9.79100000
C	4.77160000	4.81770000	14.60270000
H	5.86740000	4.83870000	14.53130000
H	4.49530000	5.12590000	15.62090000
H	4.38190000	5.57300000	13.90660000
C	2.20580000	3.12170000	14.35540000
H	1.74970000	3.87080000	13.69430000
H	1.90360000	3.36150000	15.38470000
H	1.77230000	2.14590000	14.09800000
C	4.79470000	1.83940000	15.41890000
H	4.40370000	0.83150000	15.22350000
H	4.53110000	2.10210000	16.45320000
H	5.89040000	1.78690000	15.35870000
C	5.51720000	-0.51750000	11.81740000
H	4.77350000	-1.27120000	11.50310000
H	5.17600000	-0.05790000	12.74730000
H	6.46430000	-1.05090000	12.01150000
C	6.14550000	-0.09220000	9.52950000
H	7.10460000	-0.62100000	9.66700000
H	6.30190000	0.67990000	8.76780000
H	5.41300000	-0.82320000	9.14480000
C	7.53510000	3.75430000	10.10090000
C	9.49190000	4.01940000	8.60540000
H	9.04870000	3.14180000	8.13010000
H	10.52440000	3.76920000	8.89300000
H	9.53210000	4.83960000	7.87240000
C	9.31440000	5.39420000	10.64780000
H	8.56980000	5.75360000	11.36140000
H	9.63120000	6.24710000	10.02960000
H	10.19380000	5.02980000	11.20110000
C	3.51880000	2.48370000	8.32420000
H	2.75200000	1.70150000	8.17440000
H	3.23420000	3.34070000	7.68660000
H	4.46970000	2.08940000	7.95000000
C	6.51170000	4.02690000	7.91800000
H	6.86650000	3.40850000	7.07770000
H	5.45840000	4.26110000	7.72620000
H	7.06960000	4.97400000	7.89460000
C	8.06660000	3.29840000	12.46480000
H	9.03540000	2.90200000	12.12350000
H	8.25800000	4.22350000	13.02930000
H	7.63530000	2.57630000	13.16600000
C	2.32060000	3.35240000	10.19830000
H	2.36730000	3.59590000	11.26140000
H	2.01370000	4.25790000	9.64310000

H	1.52610000	2.59720000	10.05050000

Species G2
HF energy = -1152.34499320
No imaginary frequency
Zero-point correction = 0.458172 (Hartree/Particle)
Thermal correction to Energy = 0.489927
Thermal correction to Enthalpy = 0.490871
Thermal correction to Gibbs Free Energy = 0.393836
Sum of electronic and zero-point Energies = -1151.886821
Sum of electronic and thermal Energies = -1151.855066
Sum of electronic and thermal Enthalpies = -1151.854122
Sum of electronic and thermal Free Energies = -1151.951157

Coordinates: **G2**

Ta	5.26910000	2.47980000	10.93770000
Si	4.18250000	2.79640000	14.30150000
N	4.65900000	2.59400000	12.64530000
N	5.36890000	0.46530000	10.67460000
N	3.79300000	3.36080000	9.86420000
N	6.94800000	2.84350000	9.17720000
N	7.01970000	3.70130000	11.23800000
N	8.72860000	4.37820000	9.69120000
C	4.18470000	4.63600000	14.76770000
H	5.18250000	5.07610000	14.63720000
H	3.88640000	4.78870000	15.81460000
H	3.48820000	5.20510000	14.13690000
C	2.43620000	2.09820000	14.54380000
H	1.71450000	2.60750000	13.89130000
H	2.09180000	2.21490000	15.58100000
H	2.40210000	1.02790000	14.29920000
C	5.37600000	1.87110000	15.45140000
H	5.41230000	0.80160000	15.20340000
H	5.07340000	1.95960000	16.50440000
H	6.39920000	2.26250000	15.36710000
C	4.89690000	-0.54140000	11.62490000
H	4.08440000	-1.14830000	11.18620000
H	4.52250000	-0.06480000	12.53240000
H	5.71040000	-1.23660000	11.89910000
C	5.85920000	-0.19300000	9.46530000
H	6.66800000	-0.90540000	9.70660000
H	6.25830000	0.53640000	8.75730000
H	5.05490000	-0.76710000	8.97120000
C	7.59840000	3.64600000	10.00820000
C	9.78020000	3.83780000	8.84490000
H	9.63570000	2.76300000	8.71430000
H	10.75480000	3.99200000	9.33210000
H	9.81670000	4.31470000	7.85310000

C	8.93190000	5.73320000	10.17990000
H	8.01390000	6.10280000	10.64170000
H	9.17710000	6.39500000	9.33560000
H	9.75140000	5.79850000	10.91260000
C	3.52150000	3.00710000	8.47630000
H	2.51290000	2.56960000	8.36800000
H	3.57440000	3.88960000	7.81410000
H	4.24000000	2.26650000	8.10810000
C	7.09310000	2.99230000	7.73800000
H	7.85340000	2.31850000	7.31120000
H	6.14340000	2.74430000	7.25030000
H	7.35610000	4.01990000	7.44260000
C	7.76730000	4.05960000	12.43590000
H	8.83990000	3.84270000	12.32390000
H	7.66220000	5.12300000	12.69980000
H	7.38710000	3.47510000	13.27870000
C	2.76270000	4.25200000	10.38470000
H	2.95840000	4.49180000	11.43270000
H	2.73190000	5.19620000	9.81220000
H	1.76040000	3.79150000	10.31370000

Species TSG1EH
HF energy = -1379.70156172
Imaginary frequency: 270*i*
Zero-point correction = 0.549983 (Hartree/Particle)
Thermal correction to Energy = 0.588396
Thermal correction to Enthalpy = 0.589340
Thermal correction to Gibbs Free Energy = 0.478112
Sum of electronic and zero-point Energies = -1379.151579
Sum of electronic and thermal Energies = -1379.113166
Sum of electronic and thermal Enthalpies = -1379.112222
Sum of electronic and thermal Free Energies = -1379.223450

Coordinates: **TSG1EH**

Ta	5.38330000	3.94740000	11.53300000
Si	3.91030000	3.16080000	14.64300000
N	4.64000000	3.49340000	13.10090000
N	7.37140000	3.72630000	11.75830000
N	5.31280000	2.16340000	10.25250000
N	3.69890000	3.65710000	10.03390000
N	3.39460000	1.54220000	8.92730000
C	2.47350000	1.94440000	14.40630000
H	1.71390000	2.36130000	13.73080000
H	1.97870000	1.71060000	15.35960000
H	2.82400000	0.99820000	13.97150000
C	5.19020000	2.38070000	15.80260000
H	5.60580000	1.45870000	15.37400000
H	4.74620000	2.12640000	16.77540000

H	6.02540000	3.06900000	15.98880000
C	3.26750000	4.76970000	15.39930000
H	4.07230000	5.51510000	15.42150000
H	2.89850000	4.62360000	16.42410000
H	2.44490000	5.18620000	14.80220000
C	8.11060000	3.53740000	13.00120000
H	8.64970000	2.57270000	12.99790000
H	7.42920000	3.56100000	13.85350000
H	8.85810000	4.33660000	13.13470000
C	8.25560000	3.68420000	10.59870000
H	8.99570000	4.49950000	10.63510000
H	7.68860000	3.78420000	9.66370000
H	8.80500000	2.72710000	10.54890000
C	4.10280000	2.42820000	9.70760000
C	4.06640000	0.59780000	8.04670000
H	5.09300000	0.92470000	7.86600000
H	3.54160000	0.57570000	7.08100000
H	4.08070000	-0.42580000	8.45130000
C	1.95040000	1.38750000	9.04450000
H	1.57450000	1.98590000	9.87630000
H	1.71150000	0.33380000	9.25270000
H	1.42510000	1.68170000	8.12370000
C	5.73630000	0.81030000	10.59320000
H	4.90830000	0.19920000	10.98620000
H	6.18230000	0.27510000	9.74250000
H	6.50270000	0.87950000	11.37140000
C	2.63530000	4.35300000	9.33460000
H	2.49430000	3.96160000	8.31720000
H	1.67190000	4.28880000	9.86400000
H	2.88100000	5.41640000	9.24860000
N	5.24940000	6.10420000	11.24690000
C	4.03810000	6.80100000	11.71060000
H	3.12360000	6.40680000	11.24550000
H	3.96940000	6.68610000	12.79510000
H	4.10800000	7.87480000	11.47430000
C	5.58990000	6.47400000	9.86330000
H	6.57420000	6.07000000	9.60340000
H	4.84460000	6.10330000	9.14480000
H	5.66780000	7.56410000	9.76700000
C	6.66350000	6.83640000	12.40270000
N	6.24970000	6.56990000	13.57280000
N	7.50340000	7.34930000	11.61140000
C	6.68920000	7.43670000	14.66280000
H	5.83560000	7.66890000	15.31640000
H	7.44290000	6.93490000	15.28940000
H	7.12100000	8.39020000	14.31750000
C	8.88820000	7.48630000	12.04350000
H	9.56470000	7.13590000	11.24940000

H	9.13740000	8.54280000	12.22640000
H	9.12170000	6.92310000	12.96220000

Species H

HF energy = -1379.77669281
No imaginary frequency
Zero-point correction = 0.554728 (Hartree/Particle)
Thermal correction to Energy = 0.592015
Thermal correction to Enthalpy = 0.592959
Thermal correction to Gibbs Free Energy = 0.485166
Sum of electronic and zero-point Energies = -1379.221965
Sum of electronic and thermal Energies = -1379.184678
Sum of electronic and thermal Enthalpies = -1379.183733
Sum of electronic and thermal Free Energies = -1379.291527

Coordinates: **H**

Ta	5.77670000	3.91460000	11.96730000
Si	4.59780000	2.59380000	15.03580000
N	5.23720000	3.22320000	13.55400000
N	7.61010000	3.01590000	11.79000000
N	4.96940000	2.61400000	10.35450000
N	3.81140000	4.38630000	10.97470000
N	2.74930000	2.86900000	9.43860000
C	4.53320000	0.69940000	14.95570000
H	3.91280000	0.36350000	14.11360000
H	4.11290000	0.26680000	15.87460000
H	5.53720000	0.27640000	14.81580000
C	5.69040000	3.10340000	16.50170000
H	6.71600000	2.72780000	16.38320000
H	5.30020000	2.70780000	17.45010000
H	5.74700000	4.19620000	16.59730000
C	2.84180000	3.25470000	15.31870000
H	2.83980000	4.35060000	15.39430000
H	2.39700000	2.85440000	16.24070000
H	2.18400000	2.98040000	14.48270000
C	8.33920000	2.37980000	12.88220000
H	8.41050000	1.28520000	12.73680000
H	7.84300000	2.56880000	13.83660000
H	9.37340000	2.76510000	12.94550000
C	8.25250000	2.71290000	10.51940000
H	9.28410000	3.10560000	10.47660000
H	7.68620000	3.13270000	9.68160000
H	8.31930000	1.62030000	10.35980000
C	3.80120000	3.28180000	10.22830000
C	2.96540000	2.12950000	8.20480000
H	3.99990000	2.25070000	7.87610000
H	2.30890000	2.53680000	7.42230000
H	2.74660000	1.05540000	8.30850000

C	1.36300000	3.01060000	9.86110000
H	1.31950000	3.39900000	10.88000000
H	0.87240000	2.02520000	9.85280000
H	0.79400000	3.67990000	9.19850000
C	5.05280000	1.16670000	10.20320000
H	4.12600000	0.66060000	10.51610000
H	5.27730000	0.85450000	9.17190000
H	5.86510000	0.79970000	10.83870000
C	2.90680000	5.50680000	10.80570000
H	2.47160000	5.53710000	9.79590000
H	2.07970000	5.48830000	11.53250000
H	3.45600000	6.44210000	10.96220000
N	6.67450000	5.81020000	10.39670000
C	6.13110000	6.06070000	9.05080000
H	6.53910000	5.30470000	8.36900000
H	5.04310000	5.96360000	9.07160000
H	6.39010000	7.06400000	8.68860000
C	8.14690000	5.97470000	10.37530000
H	8.55340000	5.73640000	11.36210000
H	8.58250000	5.29070000	9.64130000
H	8.40990000	7.00840000	10.10570000
C	6.13330000	6.71190000	11.43480000
N	5.99140000	5.94300000	12.56240000
N	5.91460000	7.92690000	11.09990000
C	5.81140000	6.53870000	13.88530000
H	6.17470000	5.83090000	14.63590000
H	6.38700000	7.46710000	13.98580000
H	4.75860000	6.75620000	14.11750000
C	5.26600000	8.89870000	11.96330000
H	4.77490000	9.64950000	11.33010000
H	4.50020000	8.47780000	12.63100000
H	5.99460000	9.44210000	12.58470000

Species TSHI
HF energy = -1379.74179179
Imaginary frequency: 133*i*
Zero-point correction= 0.552704 (Hartree/Particle)
Thermal correction to Energy= 0.590063
Thermal correction to Enthalpy= 0.591008
Thermal correction to Gibbs Free Energy= 0.482232
Sum of electronic and zero-point Energies= -1379.189087
Sum of electronic and thermal Energies= -1379.151728
Sum of electronic and thermal Enthalpies= -1379.150784
Sum of electronic and thermal Free Energies= -1379.259560

Coordinates: **TSHI**

Ta	5.66950000	3.86680000	12.03830000
Si	3.99660000	3.16740000	15.07910000

N	4.85220000	3.51140000	13.61550000
N	7.36130000	2.74840000	12.34400000
N	5.16130000	2.27170000	10.59560000
N	4.01510000	4.14620000	10.52010000
N	3.26230000	2.33760000	9.11280000
C	3.82140000	1.28820000	15.28850000
H	3.27120000	0.85210000	14.44350000
H	3.28080000	1.02930000	16.21010000
H	4.80450000	0.79990000	15.32920000
C	4.92590000	3.85710000	16.58360000
H	5.93120000	3.42070000	16.66210000
H	4.39490000	3.63910000	17.52110000
H	5.04510000	4.94610000	16.51100000
C	2.25680000	3.92360000	15.02520000
H	2.29440000	5.01580000	14.91990000
H	1.69130000	3.69390000	15.93960000
H	1.68730000	3.53070000	14.17200000
C	7.78040000	2.07400000	13.56170000
H	7.80070000	0.97340000	13.43460000
H	7.10040000	2.31460000	14.38110000
H	8.80270000	2.37670000	13.85770000
C	8.24900000	2.41410000	11.24180000
H	9.29370000	2.70590000	11.45520000
H	7.94140000	2.91880000	10.31730000
H	8.25320000	1.32700000	11.03400000
C	4.10650000	2.90920000	10.03800000
C	3.74670000	1.37790000	8.13230000
H	4.83760000	1.41040000	8.08960000
H	3.35950000	1.64880000	7.13910000
H	3.42800000	0.34780000	8.35450000
C	1.83510000	2.62290000	9.08270000
H	1.52810000	3.09330000	10.01880000
H	1.28340000	1.67690000	8.98570000
H	1.54880000	3.27430000	8.24290000
C	5.18600000	0.82690000	10.77670000
H	4.18280000	0.41650000	10.97370000
H	5.60630000	0.29210000	9.91120000
H	5.81920000	0.60330000	11.64000000
C	3.25240000	5.21650000	9.90250000
H	3.35980000	5.21700000	8.80530000
H	2.17860000	5.16470000	10.13600000
H	3.61590000	6.16060000	10.31350000
N	6.25470000	7.46390000	10.49580000
C	5.41740000	8.65550000	10.48390000
H	4.72590000	8.64020000	9.62770000
H	4.83090000	8.68170000	11.40260000
H	6.04150000	9.55790000	10.40530000
C	7.05660000	7.24540000	9.30030000

H	7.31750000	6.18870000	9.21380000
H	6.46860000	7.52760000	8.41540000
H	7.98070000	7.84190000	9.29740000
C	6.11950000	6.52750000	11.49000000
N	7.02520000	5.53570000	11.66980000
N	4.99130000	6.46680000	12.21640000
C	8.46730000	5.70990000	11.52840000
H	8.96110000	5.16900000	12.34350000
H	8.87130000	5.31780000	10.58280000
H	8.74360000	6.77060000	11.60020000
C	5.12710000	6.68160000	13.65980000
H	4.27720000	6.22910000	14.17710000
H	6.04930000	6.26450000	14.10100000
H	5.10980000	7.76410000	13.88350000

Species I
HF energy = -1379.78664024
No imaginary frequency
Zero-point correction = 0.553320 (Hartree/Particle)
Thermal correction to Energy = 0.591462
Thermal correction to Enthalpy = 0.592406
Thermal correction to Gibbs Free Energy = 0.481285
Sum of electronic and zero-point Energies = -1379.233320
Sum of electronic and thermal Energies = -1379.195178
Sum of electronic and thermal Enthalpies = -1379.194234
Sum of electronic and thermal Free Energies = -1379.305356

Coordinates: **I**

Ta	5.24230000	2.79170000	11.06010000
Si	4.03710000	2.75090000	14.39260000
N	4.61530000	2.64290000	12.76660000
N	5.40280000	0.81920000	10.58390000
N	3.47530000	3.13120000	9.77780000
N	4.55550000	4.90340000	10.54390000
N	2.57840000	5.30670000	9.23890000
N	6.81480000	3.32980000	9.29760000
N	7.26200000	3.46160000	11.47600000
N	8.97180000	4.17660000	9.93480000
C	3.06430000	4.36430000	14.63000000
H	3.69580000	5.23490000	14.40660000
H	2.68990000	4.47330000	15.65780000
H	2.19990000	4.40100000	13.95290000
C	2.88610000	1.29110000	14.78180000
H	2.03640000	1.26710000	14.08590000
H	2.48150000	1.35370000	15.80210000
H	3.41260000	0.33110000	14.69180000
C	5.47670000	2.72670000	15.63130000
H	6.06700000	1.80470000	15.53670000

H	5.11800000	2.78570000	16.66870000
H	6.15550000	3.57410000	15.46460000
C	5.17680000	-0.30540000	11.48680000
H	4.32080000	-0.92150000	11.15340000
H	4.97460000	0.05530000	12.49680000
H	6.05910000	-0.97030000	11.51580000
C	5.63020000	0.32980000	9.22790000
H	6.52360000	-0.31880000	9.18480000
H	5.78270000	1.16160000	8.53630000
H	4.77310000	-0.27280000	8.87500000
C	3.50990000	4.48060000	9.83810000
C	1.90360000	4.93410000	8.00670000
H	2.44890000	4.12420000	7.51670000
H	1.89040000	5.79760000	7.32540000
H	0.86240000	4.61400000	8.17080000
C	2.13100000	6.53910000	9.86870000
H	2.55490000	6.61770000	10.87180000
H	1.03400000	6.53110000	9.96250000
H	2.41620000	7.43090000	9.28950000
C	7.71440000	3.66200000	10.21100000
C	9.75240000	3.70430000	8.80350000
H	9.26300000	2.83780000	8.35370000
H	10.75130000	3.39230000	9.14610000
H	9.88550000	4.47780000	8.03080000
C	9.60980000	5.17020000	10.78160000
H	8.87590000	5.60280000	11.46520000
H	10.01000000	5.98160000	10.15490000
H	10.44270000	4.75550000	11.37150000
C	2.23140000	2.38380000	9.65990000
H	1.38860000	2.89960000	10.14690000
H	1.94670000	2.18460000	8.61510000
H	2.36050000	1.41340000	10.15070000
C	6.80990000	3.91340000	7.97100000
H	7.22150000	3.23590000	7.20450000
H	5.77160000	4.12610000	7.68220000
H	7.37520000	4.85750000	7.91600000
C	8.15370000	3.21180000	12.60040000
H	9.07820000	2.70610000	12.28170000
H	8.43930000	4.13110000	13.13490000
H	7.64210000	2.56630000	13.32020000
C	5.15510000	6.21170000	10.38600000
H	4.87260000	6.68920000	9.43550000
H	4.88610000	6.89840000	11.20440000
H	6.24740000	6.10920000	10.39990000

Nugent monomer
HF energy = -673.460923293
No imaginary frequency

Zero-point correction = 0.371925 (Hartree/Particle)
Thermal correction to Energy = 0.395436
Thermal correction to Enthalpy = 0.396381
Thermal correction to Gibbs Free Energy = 0.317783
Sum of electronic and zero-point Energies = -673.088999
Sum of electronic and thermal Energies = -673.065487
Sum of electronic and thermal Enthalpies = -673.064543
Sum of electronic and thermal Free Energies = -673.143140

Coordinates: **Nugent monomer**

Ta	6.96670000	5.09360000	3.70050000
N	8.13360000	5.65790000	5.26780000
N	5.00260000	5.35600000	4.15490000
N	7.45690000	6.16050000	2.03980000
N	7.25230000	3.35090000	3.36530000
C	4.01800000	4.34590000	4.51850000
H	3.54970000	4.57630000	5.49220000
H	3.20660000	4.28610000	3.77030000
H	4.48980000	3.36190000	4.59090000
C	4.38800000	6.67310000	4.03120000
H	3.58590000	6.67590000	3.27160000
H	3.94480000	7.00640000	4.98660000
H	5.12340000	7.43050000	3.72520000
C	7.80020000	6.83550000	6.06130000
H	7.59030000	6.56910000	7.11280000
H	8.62400000	7.57150000	6.06200000
H	6.90480000	7.33990000	5.67190000
C	9.29650000	4.96820000	5.81020000
H	9.12180000	4.63980000	6.85110000
H	9.53250000	4.08660000	5.20740000
H	10.18370000	5.62650000	5.81850000
C	7.74140000	7.58810000	2.13260000
H	7.61290000	7.95620000	3.16030000
H	8.78110000	7.81380000	1.83500000
H	7.07200000	8.17870000	1.48180000
C	7.65850000	5.66950000	0.68320000
H	6.98690000	6.18000000	-0.03030000
H	8.69490000	5.84450000	0.34120000
H	7.45710000	4.59570000	0.63280000
C	7.32860000	1.16040000	4.43400000
H	8.03180000	1.52530000	5.19280000
H	6.31170000	1.28110000	4.82790000
H	7.51250000	0.08850000	4.27820000
C	8.93450000	1.76660000	2.58170000
H	9.66680000	2.13410000	3.31140000
H	9.14850000	0.70760000	2.38250000
H	9.07290000	2.32840000	1.64970000
C	6.48560000	1.43110000	2.06910000

H	6.59170000	1.98180000	1.12610000
H	6.64420000	0.36340000	1.86460000
H	5.45760000	1.56540000	2.42720000
C	7.49640000	1.94980000	3.11630000

Nugent dimer
HF energy = -1346.89901833
No imaginary frequency
Zero-point correction = 0.751552 (Hartree/Particle)
Thermal correction to Energy = 0.796039
Thermal correction to Enthalpy = 0.796983
Thermal correction to Gibbs Free Energy = 0.679831
Sum of electronic and zero-point Energies = -1346.147466
Sum of electronic and thermal Energies = -1346.102980
Sum of electronic and thermal Enthalpies = -1346.102035
Sum of electronic and thermal Free Energies = -1346.219187

Coordinates: **Nugent dimer**

Ta	26.17200000	15.93740000	14.58600000
Ta	25.33810000	13.67280000	12.43930000
N	26.56080000	17.98460000	14.78870000
N	24.41590000	16.30790000	15.60690000
N	27.93760000	15.55720000	15.51440000
N	23.78400000	14.54440000	11.39880000
N	26.92670000	12.79460000	11.52850000
N	24.28620000	11.87430000	12.23280000
N	26.21620000	15.70360000	12.62830000
N	25.50400000	13.82950000	14.39810000
C	25.55540000	19.04550000	14.77210000
H	25.56810000	19.62210000	15.71500000
H	24.55340000	18.63300000	14.63050000
H	25.74490000	19.76840000	13.95940000
C	27.87390000	18.60970000	14.91810000
H	28.08440000	19.28460000	14.06800000
H	28.66630000	17.85890000	14.95630000
H	27.93390000	19.22830000	15.83330000
C	24.35710000	17.07400000	16.84760000
H	23.61190000	17.88730000	16.79020000
H	25.32520000	17.52490000	17.08360000
H	24.06290000	16.42780000	17.69520000
C	23.08600000	15.80590000	15.29130000
H	22.64940000	15.27360000	16.15630000
H	23.11490000	15.10630000	14.45410000
H	22.39280000	16.62860000	15.03730000
C	28.20430000	15.94780000	16.89380000
H	28.44170000	15.06940000	17.51910000
H	27.34000000	16.45140000	17.34030000
H	29.06440000	16.63720000	16.95540000

C	29.10290000	14.91080000	14.92800000
H	29.99540000	15.55850000	15.00480000
H	28.93710000	14.69500000	13.87130000
H	29.34130000	13.96400000	15.44530000
C	23.11440000	15.80180000	11.69910000
H	23.14300000	16.48250000	10.82840000
H	23.59520000	16.31400000	12.53400000
H	22.04910000	15.64430000	11.94910000
C	23.24980000	14.00010000	10.15450000
H	22.15230000	13.88300000	10.19820000
H	23.68080000	13.01980000	9.93160000
H	23.46810000	14.67350000	9.30510000
C	26.87940000	12.32880000	10.14730000
H	27.66040000	12.81400000	9.53630000
H	25.91080000	12.54750000	9.68460000
H	27.04350000	11.23870000	10.08610000
C	28.21980000	12.49630000	12.12730000
H	28.45100000	11.41770000	12.05430000
H	28.23250000	12.76930000	13.18380000
H	29.03460000	13.03970000	11.61600000
C	24.86830000	10.53990000	12.12100000
H	24.57310000	9.89910000	12.97220000
H	25.95930000	10.58640000	12.09760000
H	24.51940000	10.02690000	11.20520000
C	22.83140000	11.73170000	12.23280000
H	22.47530000	11.28100000	11.28840000
H	22.34130000	12.69960000	12.36220000
H	22.49090000	11.06620000	13.04520000
C	28.30270000	16.63740000	11.67040000
H	28.57750000	17.11090000	12.61980000
H	28.74070000	17.23330000	10.85700000
H	28.75540000	15.63860000	11.63900000
C	26.48020000	15.93820000	10.12440000
H	26.91530000	14.93950000	10.02450000
H	26.92840000	16.57460000	9.34950000
H	25.40620000	15.87280000	9.92890000
C	26.17960000	17.96890000	11.51890000
H	25.08740000	17.94480000	11.43170000
H	26.57420000	18.54090000	10.66780000
H	26.44080000	18.49560000	12.43640000
C	25.53910000	13.48700000	16.90230000
H	26.53660000	13.92410000	17.00510000
H	25.43020000	12.72070000	17.68150000
H	24.79500000	14.26720000	17.08670000
C	23.95760000	12.17490000	15.50750000
H	23.16280000	12.92560000	15.58180000
H	23.86140000	11.49410000	16.36460000
H	23.80390000	11.59920000	14.59480000

C	26.42820000	11.74300000	15.36490000
H	26.32680000	11.21280000	14.41150000
H	26.34710000	11.00310000	16.17390000
H	27.43170000	12.18390000	15.41010000
C	26.76740000	16.54290000	11.51700000
C	25.34940000	12.84000000	15.51180000

3) **Complete list of authors for reference 29 (S62)**

(31) Gaussian 09, Revision A.02: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.