Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Mechanistic Study on the Regioselective Ni-Catalyzed Dicarboxylation of 1,3-Dienes with CO_2

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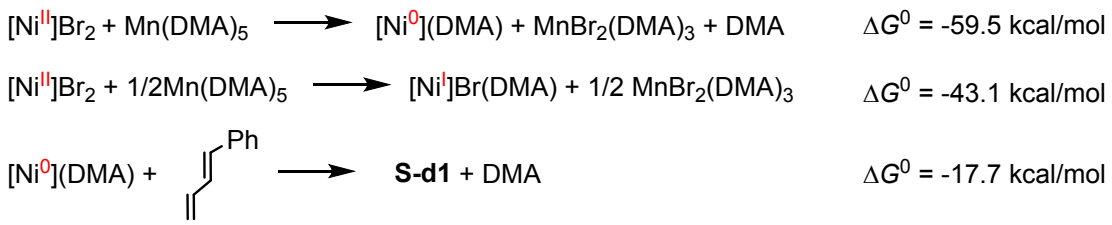

Fig. S1 Reduction of Ni(II) species to Ni(0) and Ni(I) species and the corresponding free energy changes. (**L1**)Ni is abbreviated to [Ni]. **S-d1** is the singlet C1,C2-coordinated [Ni]-diene intermediate.

The computation of $[Ni]Br_2$ (triplet) was based on the single crystal structure of the paramagnetic $[Ni]Br_2$ species reported by Martin et al. (*Angew. Chem. Int. Ed.* **2016**, 55, 11207). And the structure of $[MnBr_2(DMA)_3]$ (sextet) was based on the single crystal structure of the high-spin $MnBr_2(DMU)_3$ species (DMU = N,N′-Dimethylurea) reported by Hugel et al. (*Inorg. Chem.* **1986**, 25, 22, 3957). The possibility of $[Ni](DMA)_2$ with the 18-electron structure was also examined, but was excluded due to the automatic dissociation of one DMA during geometry optimization.

Table S1 Gibbs free energies gap between **S-d1** and **T-d1** calculated at the M(sp)-IEFPCM/SDD+f-6-311G(d,p)//B3LYP-D3-IEFPCM/SDD+f-6-311G(d,p) level of theory.

M(sp)	B3LYP-D3	M06	M06L	B3PW91	mPW-B95	PBE1PBE
Δ*G*(T-d1)-Δ*G*(S-d1) (kcal/mol)	4.2	9.5	11.2	3.3	18.4	1.0

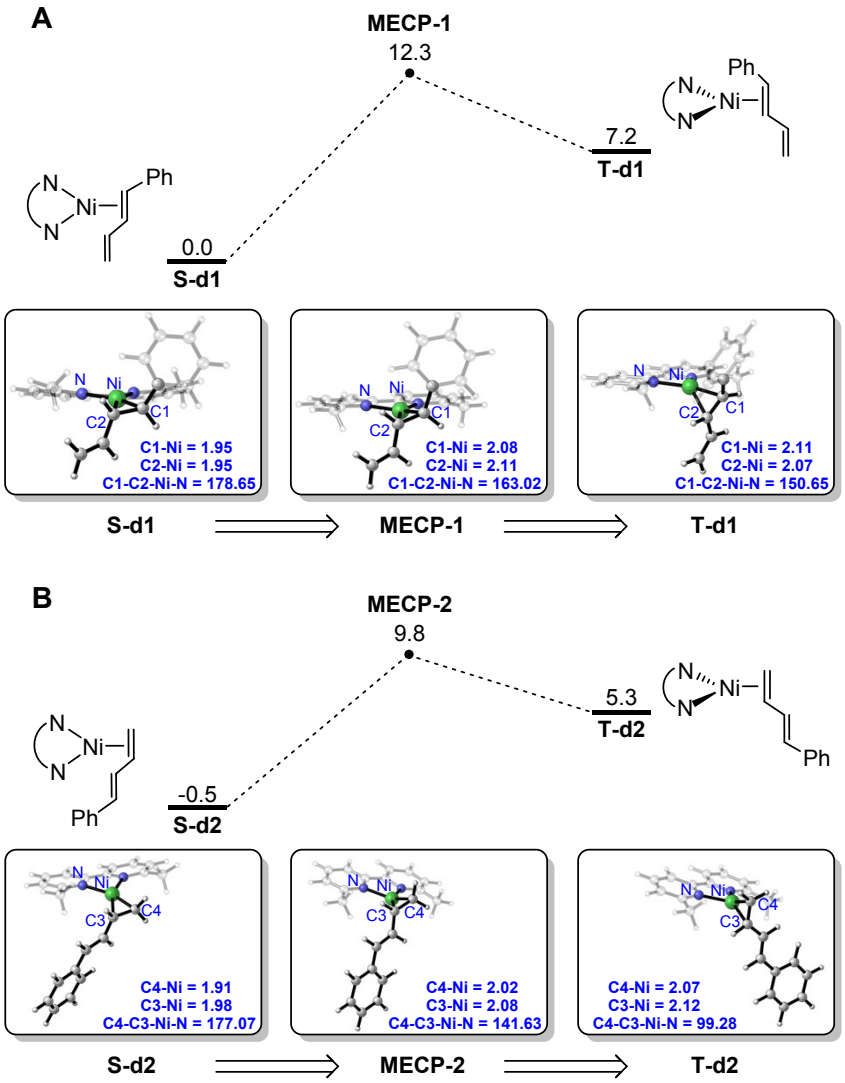

Fig. S2 Electronic energy profiles of the spin inversion progress of (A) **S-d1** and (B) **S-d2** (in kcal/mol). Bond lengths and angles are given in angstroms and degrees, respectively.

This progress is discussed with electronic energies because minimum energy crossing points (MECPs) are not stationary points and cannot be analyzed with frequency calculations.

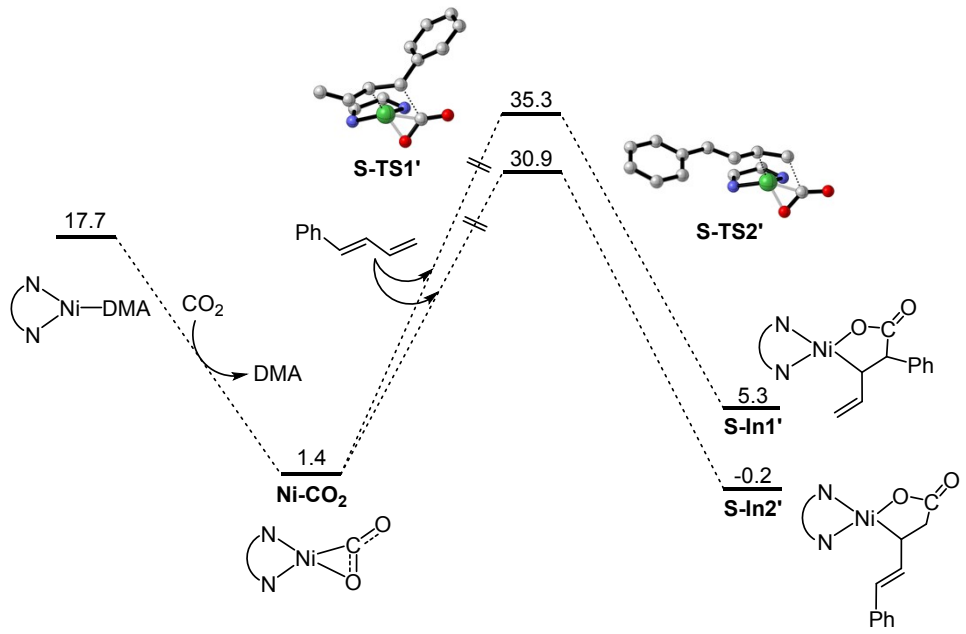

Fig. S3 Gibbs free energy profile of the typical CO_2 coordination-alkene insertion pathway starting from [Ni](DMA) (in kcal/mol).

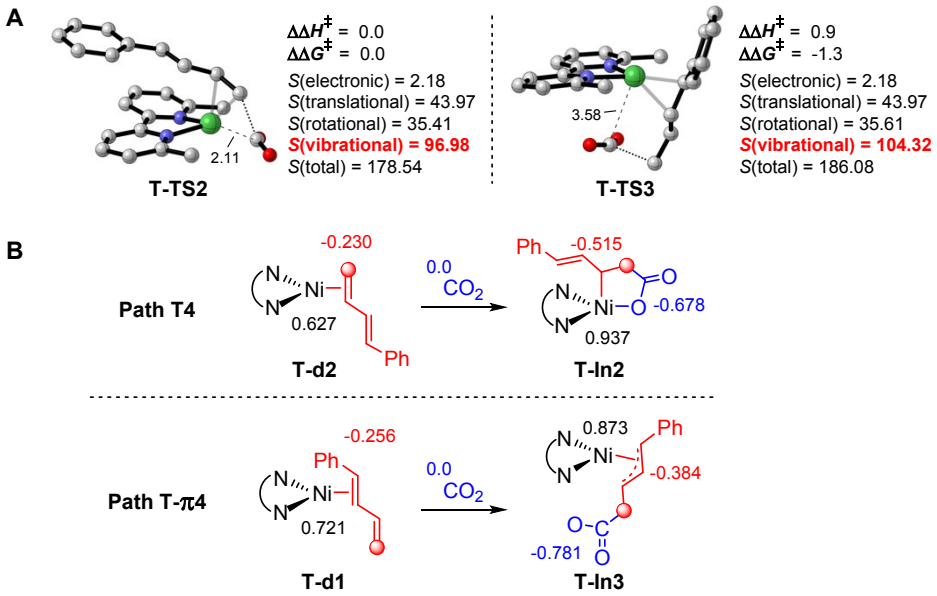

Fig. S4 (A) Optimized structures, relative Gibbs free energies/enthalpies, and entropies of **T-TS2** and **T-TS3**. Distances are given in angstroms. Energies and entropies are given in kcal/mol and cal·mol^{-1}·K^{-1}. (B) NBO charge distribution in the intermediates of Path T4/Path T-π4.

The relative enthalpy of **T-TS3** is slightly higher than **T-TS2**, but Gibbs free energy of **T-TS3** is relatively lower (Fig. S4A). In other words, the entropic effect is mainly responsible for the relatively lower free energy of **T-TS3** than **T-TS2**. From the calculation results in Fig. S4, the electronic, translational, and rotational entropy of **T-TS2** are very close to the related ones of **T-TS3**, and the two species are mainly differentiated on the vibrational entropy. After a careful analysis on the vibrational modes and the optimized geometries of **T-TS2** and **T-TS3**, we noticed that the higher confusion degree (and thus higher vibrational entropy) of CO_2 moiety in **T-TS3** than that in **T-TS2** accounts for the larger entropic effect in the former case (the C-Ni bond distance in **T-TS2** and **T-TS3** is 2.11 and 3.58 Å).

In the precursor of **T-TS2** (i.e. **T-d2** in Fig. S4B), the two coordinated C atoms (i.e. C3 and C4) feature some sp^3 characteristics due to a degree of Ni-C covalent bonding character. By contrast, in the precursor of **T-TS3** (i.e. **T-d1** in Fig. S4B), the terminal, uncoordinated atom is a typical C(sp^2). To this end, the electron transfer from the free alkene group in **T-d1** is more efficient than that of the coordinated alkene in **T-d2**, resulting in the necessity of the Ni-C bond assisted carboxylation in **T-TS2**. The C-C bond formation in **T-TS3** satisfies the electronic demand of CO_2 insertion and the vibrational motion of the CO_2 moiety is easier than that in **T-TS2**. In this context, the carboxylation occurring on the uncoordinated alkene group is more favored.

Table S2 Gibbs free energies gap between **S-TS3** and **T-TS3** with the full ligand calculated at the M(sp)-IEFPCM/SDD+f-6-311G(d,p)//B3LYP-D3-IEFPCM/SDD+f-6-311G(d,p) level of theory.

M(sp)	B3LYP-D3	B3LYP*
Δ*G*(S-TS3)-Δ*G*(T-TS3) (kcal/mol)	5.1	8.1

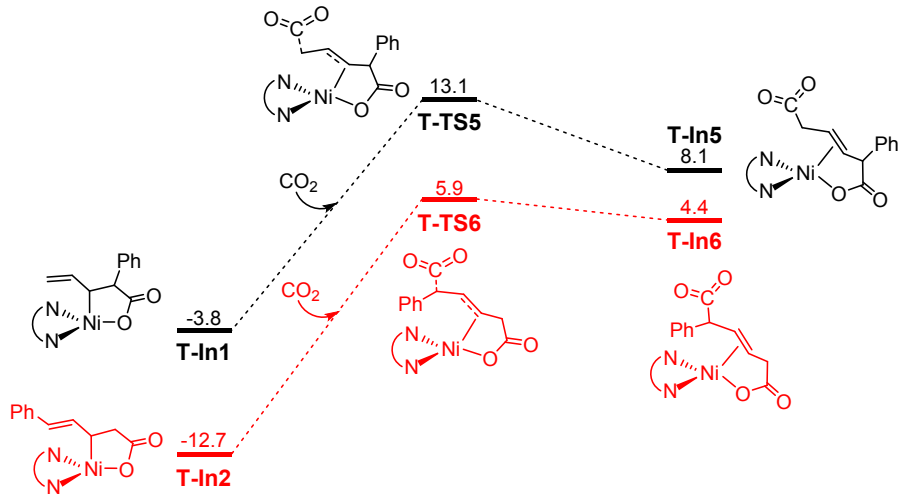

Fig. S5 Gibbs free energy profile of the direct carboxylation of Ni(II) species (in kcal/mol).

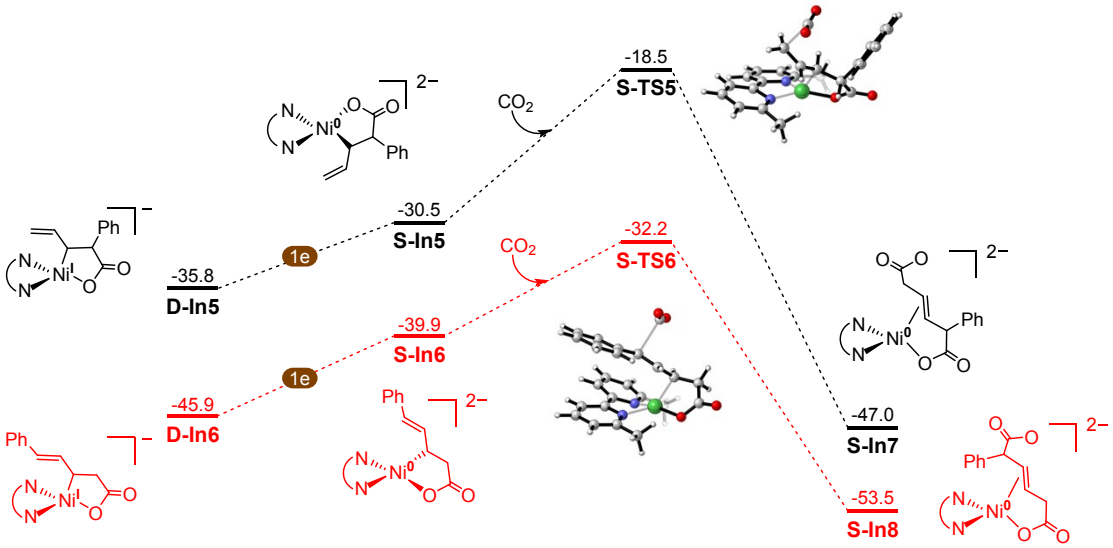

Fig. S6 Gibbs free energy profiles of one-electron reduction of Ni(I) species and carboxylation of Ni(0) species (in kcal/mol).

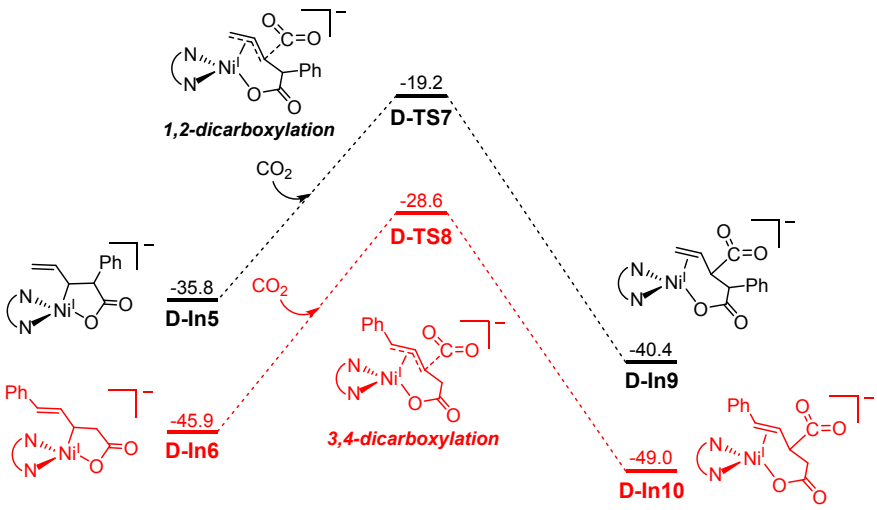

Fig. S7 Gibbs free energy profiles of 1,2 and 3,4-dicarboxylation (in kcal/mol).

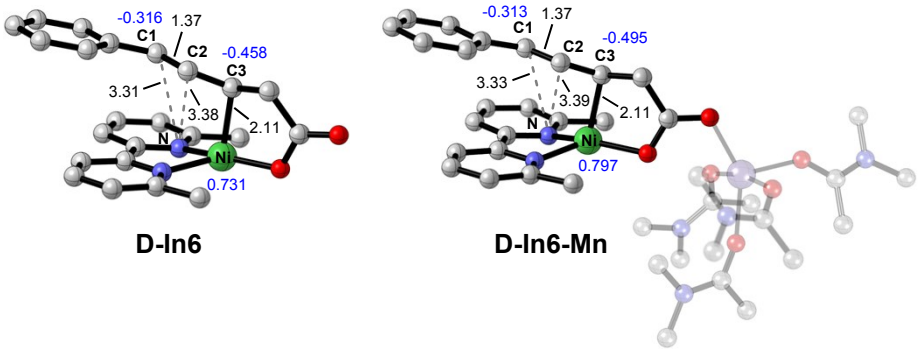

Fig. S8 Optimized structures and NBO charge distribution (blue color) of **D-In6** and **D-In6-Mn**. Bond distances are given in angstroms (black color).

D-In6 + $[Mn(DMA)_5]^{2+}$ → **D-In6-Mn** + DMA ΔG^o = -10.2 kcal/mol (S1)

After reduction of the alkyl-Ni(II) intermediate, no bromide is available and thus $[Mn(DMA)_5]^{2+}$ was used as the Mn(II) product to keep consistency on the number of ligands with $MnBr_2(DMA)_3$. The reaction of **D-In6** with $[Mn(DMA)_5]^{2+}$ is exergonic by 10.2 kcal/mol (eq. S1). Albeit the thermodynamic feasibility, the binding of $[Mn(DMA)_5]^{2+}$ makes little influence on the electronic and steric effect on the reaction center of **D-In6**. For example, the C1-C2 and C3-Ni bond lengths, and NBO charges on C1, C3, Ni of **D-In6-Mn** are all quite close to the related ones of **D-In6** (Fig. S8). Meanwhile, the C1/C2-N bond lengths in **D-In6** are also close to the related ones in **D-In6-Mn**, verifying the similar chemical environment of the C1=C2 double bond. In view of the great similarity of the Mn-absent and Mn-present systems, and the especially time-consuming calculations on the Mn-present molecules, the subsequent transformations from **D-In6** was conducted.

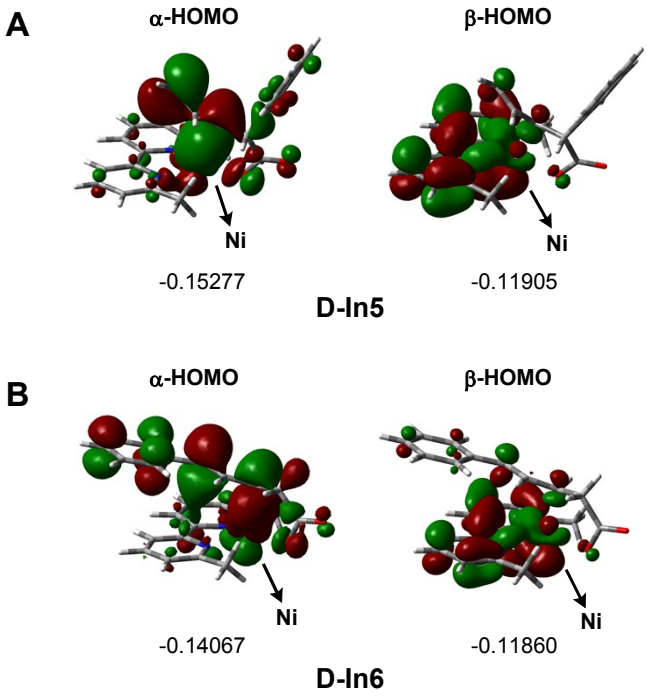

Fig. S9 The frontier molecular orbital of (A) **D-In5** and (B) **D-In6**.

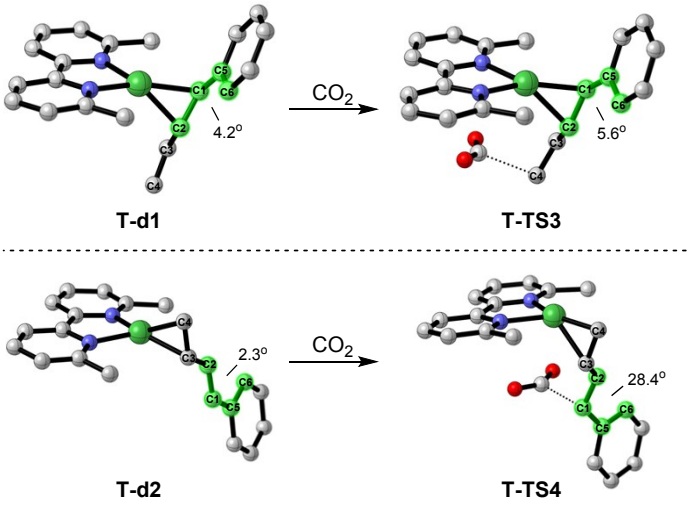

Fig. S10 Optimized structures of **T-d1**, **T-d2**, **T-TS3** and **T-TS4**.

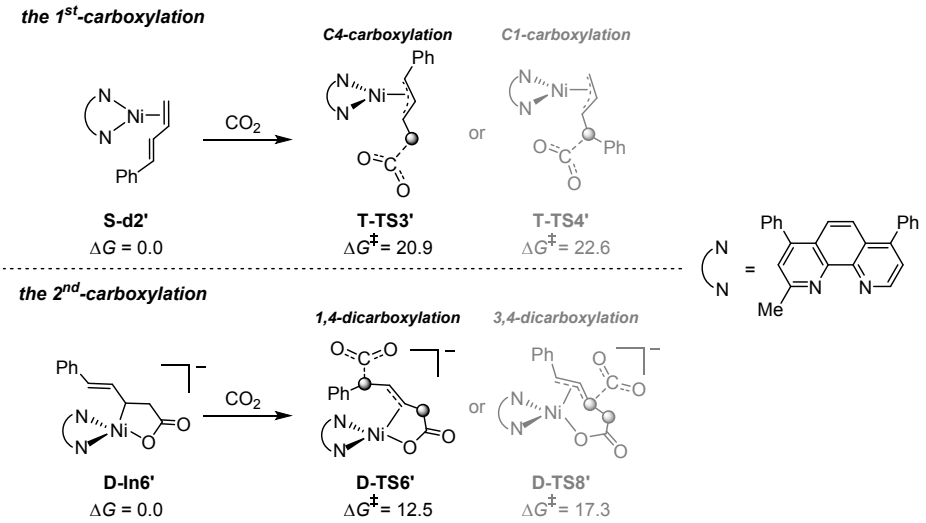

Fig. S11 Relative Gibbs free energies of the key intermediates and transition states with the full ligand (in kcal/mol).

Similar to the modeling reaction system, the calculation results indicate that the first carboxylation occurs favorably on the C4-position (over the C1-position); and the second carboxylation selectivity on the C1-position (instead of the C3-position). In this context, the 1,4-dicarboxylation is the predicted product of the reaction system with 2-methyl-4,7-diphenyl-1,10-phenanthroline, and the first carboxylation step is the rate-determining step.

Cartesian coordinates of all intermediates and transition states

[Ni]Br_2 (triplet)

Thermal Correction to Free Energy: 0.168464 Hartree
SCF energy: -5893.647546 Hartree
Gibbs free energy: -5893.479082 Hartree
Coordinates:

C	-2.66210200	0.57469600	-0.11861400
C	-0.74191700	1.92073700	-0.03246500
C	-1.50996100	3.08187500	-0.05762600
C	-2.89424100	2.96762100	-0.11336900
C	-3.47659700	1.70777300	-0.14362700
H	-1.04674400	4.05713700	-0.03397300
H	-3.51149400	3.85725600	-0.13243700
H	-4.55133700	1.59125200	-0.18612500
C	0.73968600	1.92149000	0.03160300
C	1.50650600	3.08345000	0.05607300
C	2.89090000	2.97068500	0.11194000
H	1.04227600	4.05822100	0.03181500
C	2.66125100	0.57749400	0.11867400
C	3.47454700	1.71146400	0.14299000
H	3.50722600	3.86097600	0.13047800
H	4.54940900	1.59610000	0.18559400
N	-1.32468500	0.70196100	-0.06420700
N	1.32368900	0.70330300	0.06414300
C	-3.21574500	-0.81722400	-0.15006100
H	-2.82761300	-1.34992800	-1.02304500
H	-2.88684000	-1.36710700	0.73636500
H	-4.30400500	-0.81346700	-0.18732800
C	3.21657200	-0.81377100	0.15092200
H	2.82880200	-1.34657600	1.02399800
H	2.88863600	-1.36443200	-0.73538700
H	4.30481100	-0.80862000	0.18853000
Ni	0.00012400	-0.83118600	0.00036200
Br	-0.15563700	-1.59611000	2.28907200
Br	0.15677000	-1.59648300	-2.28822900

$Mn(DMA)_5$ (quartet)

Thermal Correction to Free Energy: 0.570196 Hartree
SCF energy: -1544.045526 Hartree
Gibbs free energy: -1543.475330 Hartree
Coordinates:

Mn	0.07403700	0.31165400	0.38508000
N	3.75018200	1.05641700	-1.72980400

C	5.01160700	0.46338100	-2.15392100
H	5.75745800	0.55789600	-1.35781500
H	4.89783700	-0.58763000	-2.39804400
H	5.38685300	0.98655200	-3.03817100
C	3.82025900	2.48121300	-1.42019300
H	2.84316200	2.82971500	-1.10123300
H	4.54525800	2.65201400	-0.61867200
H	4.13937900	3.03864500	-2.30558900
C	2.60730400	0.36482000	-1.52492300
C	2.57540800	-1.11480100	-1.83774500
H	2.81881200	-1.29788000	-2.88809700
H	3.27095800	-1.66853300	-1.20635300
H	1.56589000	-1.46187200	-1.63795100
O	1.56786200	0.95696500	-1.15647200
N	-1.94784200	3.24148200	-0.61591400
C	-3.29657700	3.78572800	-0.74084800
H	-3.92383800	3.07108100	-1.28027200
H	-3.74696700	3.96627200	0.22950400
H	-3.27465500	4.72400900	-1.30270700
C	-1.33058700	2.83937600	-1.88001000
H	-0.31115800	2.50728900	-1.70397800
H	-1.90188700	2.02177400	-2.32954600
H	-1.33164200	3.68743400	-2.56990700
C	-1.28820800	3.08201000	0.54821800
C	-1.93989000	3.53908100	1.83189800
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H	-2.77846700	2.88091000	2.07145700
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O	-0.15535500	2.55555800	0.58218400
N	3.62684600	-1.67412500	1.56444200
C	5.05778000	-1.53677000	1.35532000
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H	5.24390300	-1.03123000	0.40573200
H	5.57014800	-0.96689400	2.15149400
C	3.31902100	-2.38072900	2.81236200
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H	3.73502500	-3.39287700	2.78504200
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H	-2.11739200	-2.53653400	-3.98745600
H	-3.51642200	-1.81807700	-3.16138800
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H	0.14707500	-2.57920000	0.55746000
H	-1.54443500	-2.86295600	0.97560600

[Ni](DMA)

Thermal Correction to Free Energy: 0.296325 Hartree

SCF energy: -1033.111195 Hartree

Gibbs free energy: -1032.814870 Hartree

Coordinates:

C	0.67994700	-2.53180900	-0.42765800
C	-1.37359800	-1.56542900	0.13338900
C	-1.93463400	-2.81406800	0.39182500
C	-1.15022600	-3.94989200	0.24681000
C	0.16342900	-3.80376600	-0.18072900
H	-2.97339200	-2.90011900	0.67718300
H	-1.56325500	-4.93215600	0.44066600
H	0.79583200	-4.66917500	-0.33141400

C	-2.15516600	-0.31281000	0.18351800
C	-3.41816600	-0.21547800	0.76603200
C	-4.07856200	1.00612400	0.72481200
H	-3.87235400	-1.06655400	1.25366100
C	-2.19271900	1.93480900	-0.45344700
C	-3.46558100	2.08631800	0.10011300
H	-5.05921300	1.11284600	1.17251700
H	-3.96314700	3.04585700	0.03887200
N	-0.07198800	-1.42095900	-0.24138900
N	-1.54755800	0.75090200	-0.39395100
C	2.08484700	-2.35221100	-0.91459200
H	2.10473800	-1.66360000	-1.75974600
H	2.69999800	-1.91017200	-0.13053300
H	2.52125900	-3.30650100	-1.21131200
C	-1.48865700	3.06740000	-1.13908500
H	-0.52403900	3.24978100	-0.66188300
H	-1.27463500	2.79869100	-2.17750400
H	-2.09271300	3.97484300	-1.12554000
Ni	0.46776200	0.42507600	-0.48363800
N	2.77692500	1.26420500	1.14054000
C	1.82548100	1.88175400	2.05907300
H	2.32307100	2.07655700	3.01235000
H	1.46322400	2.82009500	1.64471000
H	0.94790700	1.23589200	2.24733300
C	3.32984300	0.04684700	1.72311800
H	4.09650900	-0.38403300	1.07936900
H	3.79943300	0.28139300	2.68187900
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H	4.07966300	1.66458600	-1.25851000
O	1.37587200	2.01834700	-0.60557500

[Ni]Br(DMA)

Thermal Correction to Free Energy: 0.285849 Hartree

SCF energy: -3607.370680 Hartree

Gibbs free energy: -3607.084831 Hartree

Coordinates:

C	1.11173600	-1.34189900	1.79459100
C	-0.96307400	-1.85904600	0.83490400
C	-0.92351400	-3.15067600	1.36396700
C	0.17203200	-3.53326400	2.12439500

C	1.19967300	-2.61942400	2.34334400
H	-1.73108300	-3.84654600	1.18691600
H	0.22415400	-4.53053200	2.54406800
H	2.06509300	-2.88849000	2.93534200
C	-2.06938800	-1.34981700	0.00335600
C	-3.18909900	-2.10761800	-0.34512500
C	-4.16570800	-1.53897300	-1.14996700
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H	-2.41579000	2.53690000	-0.82034900
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H	-3.44370400	2.28486200	-2.25656800
Ni	-0.24094700	0.81804400	0.17308300
N	3.31211200	-0.40624900	-1.65006600
C	3.94303500	-1.59265400	-2.22387600
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H	3.25369800	-2.43067600	-2.26105600
H	4.31221000	-1.38711900	-3.23387400
C	4.23616200	0.64854400	-1.23478900
H	4.80042000	1.01328500	-2.09840900
H	3.67520300	1.46840300	-0.79709200
H	4.94039100	0.25187100	-0.49934600
C	1.97867100	-0.19707400	-1.61960500
C	1.06108200	-1.28239600	-2.14057800
H	1.31741800	-1.57375000	-3.16071000
H	1.10969700	-2.17169200	-1.50764600
H	0.04475700	-0.89705600	-2.11458400
O	1.50529100	0.86242700	-1.15976700
Br	-0.04758000	3.03559900	1.19318700

$MnBr_2(DMA)_3$ (sextet)

Thermal Correction to Free Energy: 0.325294 Hartree

SCF energy: -6116.726477 Hartree

Gibbs free energy: -6116.401184 Hartree

Coordinates:

Mn	-0.27191100	-0.64911500	-0.08634300
N	-3.96411000	1.63105900	0.36513700
C	-3.38201900	2.96101800	0.17761800
H	-3.97842900	3.68692300	0.73247800
H	-2.36112700	2.96901900	0.54748900
H	-3.38297800	3.23725800	-0.88084000
C	-5.42611800	1.57963600	0.36814600
H	-5.78869500	0.57232700	0.18723000
H	-5.82395800	1.94252800	1.32032300
H	-5.79917500	2.22046600	-0.43302600
C	-3.16797200	0.55958000	0.49183200
C	-3.78027400	-0.79022300	0.77559400
H	-4.17378700	-1.21909300	-0.14918800
H	-2.99659900	-1.44490500	1.15131000
H	-4.58550500	-0.73398300	1.50828600
O	-1.92457800	0.68669200	0.38424100
N	2.29462300	2.87146300	0.45508700
C	3.21460100	2.24137900	1.40440300
H	3.10302700	2.69377900	2.39382700
H	3.00236700	1.17875800	1.46614400
H	4.24016100	2.39230600	1.06206200
C	2.60101700	4.26207700	0.12526400
H	1.95879900	4.63478400	-0.66574800
H	2.47789900	4.89356300	1.00992000
H	3.63772000	4.33060800	-0.21091200
C	1.20207500	2.21516900	0.03433800
C	0.24891100	2.88314700	-0.92728100
H	0.74381300	3.10087600	-1.87638700
H	-0.58491000	2.20706500	-1.09571400
H	-0.13527700	3.82105100	-0.52214200
O	0.98779200	1.04282300	0.41984400
N	3.78633600	-1.03165600	-0.24560000
C	5.10899100	-0.48125800	-0.53324100
H	5.82658300	-1.29871800	-0.64008900
H	5.10900100	0.09846300	-1.45047600
H	5.43149600	0.16052400	0.29057600
C	3.71573500	-1.92942000	0.90993300
H	2.68301900	-2.02592700	1.23581300
H	4.11164800	-2.91631000	0.65245200
H	4.31867400	-1.50848500	1.71631200
C	2.69698500	-0.83274200	-0.99922400
C	2.74804500	0.14790000	-2.14803000
H	3.36426900	-0.24091700	-2.96240400

H	1.73284200	0.28311400	-2.51439700
H	3.15553100	1.11345100	-1.84489400
O	1.63433400	-1.45258400	-0.75717600
Br	-0.25617100	-1.93036200	2.20066800
Br	-1.56002500	-1.53620200	-2.21047400

DMA

Thermal Correction to Free Energy: 0.096379 Hartree
SCF energy: -287.929558 Hartree
Gibbs free energy: -287.833179 Hartree
Coordinates:

N	-0.58805500	0.07820500	-0.03779500
C	-1.63225000	-0.93942100	0.00546300
H	-2.31146000	-0.81746600	-0.84368400
H	-1.17217500	-1.92238800	-0.03609300
H	-2.21407600	-0.85019500	0.92928800
C	-1.06986700	1.45322200	0.01063100
H	-0.27186300	2.16557800	-0.17444900
H	-1.83713900	1.59818400	-0.75528800
H	-1.51612600	1.67412200	0.98701800
C	0.72404300	-0.29365300	-0.00633900
C	1.77064600	0.81033500	0.00232500
H	1.66362100	1.46129500	0.87331400
H	2.74831200	0.33413300	0.03235500
H	1.70667600	1.43363500	-0.89291900
O	1.07064700	-1.47590300	0.00906700

1-Phenyl-1,3-butadiene

Thermal Correction to Free Energy: 0.131537 Hartree
SCF energy: -387.169928 Hartree
Gibbs free energy: -387.038392 Hartree
Coordinates:

C	1.97702600	0.13842400	-0.00004400
H	1.85608800	1.21923400	-0.00008600
C	0.89673800	-0.66754600	-0.00001200
H	1.06883200	-1.74249400	0.00007000
C	3.34195000	-0.35231000	0.00000000
H	3.46905100	-1.43355400	0.00000900
C	4.42716600	0.43488500	0.00002800
H	4.34063300	1.51730100	0.00001900
H	5.42835800	0.02080800	0.00005800
C	-0.51277700	-0.26845800	-0.00002400
C	-1.50032000	-1.26997100	-0.00000500
C	-0.93762900	1.07404900	0.00000700

C	-2.85504200	-0.94882500	0.00001500
H	-1.19608100	-2.31162900	0.00000700
C	-2.28982700	1.39407700	0.00000800
H	-0.20821700	1.87529300	0.00002300
C	-3.25703900	0.38573600	0.00000300
H	-3.59578500	-1.74056600	0.00002300
H	-2.59365800	2.43501000	0.00001000
H	-4.31069900	0.64023500	0.00000600

CO_2

Thermal Correction to Free Energy: -0.009077 Hartree
SCF energy: -188.643855 Hartree
Gibbs free energy: -188.652931 Hartree
Coordinates:

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16036900
O	0.00000000	0.00000000	-1.16036900

S-d1

Thermal Correction to Free Energy: 0.329444 Hartree
SCF energy: -1132.377800 Hartree
Gibbs free energy: -1132.048356 Hartree
Coordinates:

C	-2.34708300	-1.91265800	0.84047100
C	-2.70156000	0.34294200	0.34803100
C	-4.06377700	0.22959400	0.62169400
C	-4.57150000	-1.00334100	1.00918200
C	-3.70246900	-2.07834700	1.13411900
H	-4.71855400	1.08560900	0.54931100
H	-5.62643100	-1.11706600	1.22709300
H	-4.06123700	-3.04663900	1.45864100
C	-2.05397600	1.63096700	0.00786800
C	-2.77178400	2.81464800	-0.15470400
C	-2.08078600	3.99332900	-0.40233900
H	-3.84996500	2.82357900	-0.08871500
C	-0.02498500	2.74024400	-0.31322000
C	-0.69508000	3.95636200	-0.46545600
H	-2.61634200	4.92582000	-0.53250000
H	-0.12306900	4.85965500	-0.63446100
N	-1.86395400	-0.72130200	0.42620700
N	-0.70036900	1.58936600	-0.10023900
C	-1.38666100	-3.05533700	0.97125700
H	-1.09549700	-3.40895000	-0.01944300
H	-0.47719200	-2.72867300	1.47657900

H	-1.83569900	-3.88129200	1.52381700
C	1.46914600	2.67429100	-0.38406800
H	1.86391700	2.06537500	0.42888100
H	1.78154800	2.19055100	-1.31166200
H	1.90853200	3.67140900	-0.34199200
Ni	-0.02786700	-0.30878500	-0.26175200
C	0.97366200	-1.81565100	-0.97969800
H	1.27483400	-2.58413900	-0.26613400
C	1.74712100	-0.58631300	-1.02549800
H	1.88587700	-0.13174900	-2.00954300
C	0.34788100	-2.32700300	-2.19699300
H	0.13845900	-1.57634300	-2.95959500
C	-0.00327700	-3.59944700	-2.45196700
H	0.19285700	-4.39636800	-1.74001000
H	-0.49275400	-3.87934900	-3.37814200
C	2.89128800	-0.36481000	-0.11933300
C	2.91772800	-0.86505300	1.19905800
C	4.00391900	0.38780500	-0.53923300
C	3.99527400	-0.62397600	2.04555900
H	2.06707600	-1.43009700	1.56391700
C	5.08157900	0.63465400	0.30839800
H	4.01629200	0.78776400	-1.54838500
C	5.08718600	0.13019400	1.60897600
H	3.98081500	-1.02032100	3.05572500
H	5.92163500	1.22104500	-0.04955100
H	5.92436400	0.32115900	2.27083200

T-d1

Thermal Correction to Free Energy: 0.324632 Hartree
SCF energy: -1132.366318 Hartree
Gibbs free energy: -1132.041686 Hartree
Coordinates:

C	-0.64220400	-2.76255000	0.05347800
C	-2.32976300	-1.14425600	0.43706800
C	-3.28233000	-2.17570500	0.60448600
C	-2.89665700	-3.49092600	0.50088400
C	-1.54432100	-3.79538600	0.22276100
H	-4.31547700	-1.93141700	0.81147500
H	-3.62121400	-4.28652600	0.62967300
H	-1.21013200	-4.82150300	0.13974500
C	-2.62531000	0.25764200	0.55254900
C	-3.89342700	0.75971400	0.92263000
C	-4.08619700	2.11340300	1.05669900
H	-4.71032000	0.07663300	1.11245500

C	-1.77146000	2.46238500	0.46837400
C	-2.99763200	2.98585300	0.83444600
H	-5.05520400	2.50573500	1.34225700
H	-3.11128500	4.05606600	0.94938800
N	-1.01184400	-1.45894300	0.15843600
N	-1.57150900	1.12668500	0.30651600
C	0.80296200	-3.02714900	-0.26159300
H	1.04395500	-2.66148500	-1.26409700
H	1.45323100	-2.49671800	0.43974600
H	1.03400400	-4.09165400	-0.21965800
C	-0.59376100	3.36630300	0.23759300
H	0.25948400	3.03756800	0.83580100
H	-0.28735100	3.34270700	-0.81108100
H	-0.83183800	4.39744200	0.49915700
Ni	0.10365300	0.13202100	-0.20401700
C	1.25040400	0.42641200	-1.89989300
H	1.59863000	-0.56835400	-2.17148400
C	1.86188200	1.10295900	-0.83683600
H	1.68237800	2.16910700	-0.75086900
C	0.40760200	1.08308600	-2.89149000
H	0.13459200	2.11461500	-2.68445000
C	-0.03761900	0.50104800	-4.01443000
H	0.21070500	-0.52834900	-4.25386300
H	-0.66307200	1.03614000	-4.71856900
C	2.95767700	0.59542000	0.00309700
C	3.59955200	-0.63789300	-0.21867000
C	3.39142900	1.37375200	1.09389400
C	4.61503800	-1.07692100	0.62478700
H	3.30834900	-1.25709100	-1.05804300
C	4.40842900	0.93459200	1.93378000
H	2.91480400	2.33051600	1.28085100
C	5.02480000	-0.29765700	1.70785400
H	5.09336800	-2.03087000	0.43195400
H	4.72165200	1.55420000	2.76682400
H	5.81737700	-0.64229400	2.36178900

S-d2

Thermal Correction to Free Energy: 0.327172 Hartree

SCF energy: -1132.378639 Hartree

Gibbs free energy: -1132.051468 Hartree

Coordinates:

C	0.10042100	2.04604800	1.32812900
C	1.84066100	1.69755600	-0.19124400
C	1.84781000	3.04323400	-0.55398000

C	0.93793400	3.90485100	0.04540100
C	0.06828300	3.40463100	1.00489300
H	2.55420600	3.42064200	-1.27907400
H	0.92195200	4.95477800	-0.22064700
H	-0.63468200	4.05496100	1.50946500
C	2.82060500	0.71540700	-0.71057600
C	3.78374100	1.03902800	-1.66399600
C	4.71470400	0.07703900	-2.03363300
H	3.81412200	2.02240900	-2.11026900
C	3.66910200	-1.45063100	-0.49007400
C	4.66697400	-1.17022100	-1.42688300
H	5.47342800	0.30381700	-2.77265200
H	5.39418300	-1.93356600	-1.67206400
N	0.95759000	1.20409300	0.71280200
N	2.74342000	-0.52410300	-0.15831700
C	-0.81700700	1.47403700	2.36514300
H	-1.60630100	0.89437900	1.88236900
H	-0.27036000	0.79027600	3.01595000
H	-1.27392600	2.26355500	2.96278100
C	3.60168800	-2.79503500	0.17230000
H	3.36799400	-2.68440400	1.23107300
H	2.80192400	-3.39487200	-0.26785000
H	4.54436500	-3.33147300	0.05624000
Ni	1.00975700	-0.79580300	0.79564600
C	-1.70019600	-1.48568600	0.44911200
H	-1.47450300	-1.67506500	-0.59953400
C	-2.92160400	-0.99447400	0.77466000
H	-3.14896300	-0.85712100	1.83066400
C	-0.61661500	-1.77557500	1.36487900
H	-0.85363300	-1.66455900	2.42411400
C	0.49008000	-2.62297900	0.98223700
H	0.41993900	-3.18236600	0.04542200
H	0.99740700	-3.18713600	1.76578200
C	-3.99577800	-0.62617200	-0.14441600
C	-5.25150100	-0.25121200	0.37604800
C	-3.85314600	-0.61406600	-1.54873700
C	-6.30966200	0.10443400	-0.45544700
H	-5.39210400	-0.24367200	1.45258100
C	-4.91160200	-0.26206100	-2.37813100
H	-2.90105900	-0.87557600	-1.99609500
C	-6.15011500	0.09974800	-1.84115500
H	-7.26228900	0.38642100	-0.01944800
H	-4.76895500	-0.26316400	-3.45375100
H	-6.97168000	0.37690800	-2.49172100

T-d2

Thermal Correction to Free Energy: 0.323991 Hartree

SCF energy: -1132.369275 Hartree

Gibbs free energy: -1132.045283 Hartree

Coordinates:

C	0.41566800	2.50426700	-0.55882600
C	2.39788400	1.54668900	0.31499900
C	2.86279400	2.82899500	0.67564800
C	2.09155400	3.93837600	0.41475300
C	0.83503500	3.77273800	-0.20948200
H	3.82150800	2.94175300	1.16356100
H	2.44008200	4.92646900	0.69108500
H	0.19984300	4.62472400	-0.41527600
C	3.11244700	0.32239200	0.57251900
C	4.38005400	0.27390600	1.19086000
C	4.98205000	-0.93956800	1.42891100
H	4.87800700	1.18978000	1.47901200
C	3.07258900	-2.03514100	0.44061100
C	4.30893000	-2.12131800	1.05573400
H	5.95547700	-0.98763600	1.90264200
H	4.74619900	-3.09297500	1.24640800
N	1.17774100	1.40219200	-0.31769400
N	2.47610200	-0.84145600	0.17846900
C	-0.91271300	2.26581100	-1.21714400
H	-1.45778000	3.19700200	-1.37195500
H	-0.77533200	1.77697100	-2.18689300
H	-1.52390100	1.59821800	-0.60248200
C	2.32308800	-3.27740600	0.05048300
H	1.36061400	-3.31458700	0.56685300
H	2.12073100	-3.28754400	-1.02225500
H	2.88792200	-4.17420400	0.30518600
Ni	0.76369200	-0.45590100	-0.82021500
C	-1.92308500	-1.24312900	-0.97522500
H	-2.18297700	-0.48407600	-1.70753200
C	-0.68193500	-1.94791700	-1.21681900
H	-0.46744300	-2.78749400	-0.56202400
C	0.13042700	-1.72120800	-2.32881300
H	-0.21437900	-1.06834600	-3.12799800
H	0.90953500	-2.42203600	-2.60103000
C	-2.74020700	-1.47119100	0.08117300
H	-2.44815400	-2.24553200	0.78770700
C	-3.98218400	-0.77301700	0.39267400
C	-4.72729000	-1.16984800	1.52056800

C	-4.48175200	0.29944700	-0.37615100
C	-5.91553300	-0.53203900	1.86366200
H	-4.36334400	-1.99029200	2.13055000
C	-5.66812600	0.93461600	-0.03210000
H	-3.93865000	0.64131800	-1.24898100
C	-6.39478200	0.52426100	1.08904000
H	-6.46813300	-0.85982600	2.73722300
H	-6.02978000	1.75693100	-0.63962800
H	-7.31978900	1.02316700	1.35397800

S-TS1

Thermal Correction to Free Energy: 0.339283 Hartree
SCF energy: -1320.985834 Hartree
Gibbs free energy: -1320.646551 Hartree
Coordinates:

C	-2.38485000	-1.96917400	0.99170800
C	-2.80840800	0.21606500	0.25420800
C	-4.17806200	-0.01501100	0.21978400
C	-4.65467300	-1.27492000	0.56584400
C	-3.75616600	-2.24132500	0.99034900
H	-4.86475000	0.77508800	-0.04702700
H	-5.71735200	-1.48216400	0.54304000
H	-4.10069200	-3.20917200	1.33094000
C	-2.20140500	1.55715800	0.09291800
C	-2.92623600	2.71586200	-0.15571400
C	-2.25748600	3.93724600	-0.11577900
H	-3.98633700	2.68033300	-0.36151600
C	-0.22260100	2.76387600	0.42368800
C	-0.91008000	3.96454500	0.20676000
H	-2.79567600	4.85747300	-0.30742100
H	-0.37762800	4.90304000	0.29508100
N	-1.92621500	-0.77597300	0.56416600
N	-0.86414900	1.58928900	0.31774000
C	-1.40860400	-2.98076000	1.50919300
H	-0.53094300	-2.48382300	1.91964600
H	-1.87677500	-3.58846000	2.28468600
H	-1.08388200	-3.64626000	0.70886000
C	1.22561200	2.76997500	0.81745700
H	1.57435100	1.76775600	1.05858300
H	1.84170000	3.14817000	0.00189300
H	1.36266000	3.41641200	1.68853500
Ni	-0.18474700	-0.25772900	-0.07974900
C	0.04393800	-2.54544600	-1.76357700
H	-0.23547200	-1.91234000	-2.60136300

C	0.70572500	-1.84243500	-0.65322400
H	0.99301200	-2.50327000	0.16466800
C	1.77400400	-0.84453400	-1.03147900
C	1.18820900	0.63128800	-1.81890600
O	2.02161500	1.52653900	-1.83268400
O	0.09322700	0.48005800	-2.39216600
C	-0.23324300	-3.85489500	-1.80984200
H	-0.74674900	-4.29499600	-2.65755100
H	0.05355600	-4.53005300	-1.00878600
H	2.20370800	-1.13977700	-1.99318600
C	2.88749700	-0.60029700	-0.05301000
C	4.15808300	-0.24773900	-0.52688300
C	2.70735600	-0.68953500	1.33432400
C	5.20901000	0.01042400	0.34953400
H	4.31580000	-0.16266600	-1.59579200
C	3.75642100	-0.43433400	2.21578100
H	1.73365100	-0.95027600	1.73557900
C	5.01358200	-0.08060400	1.72789800
H	6.18221700	0.28312800	-0.04408600
H	3.58815000	-0.50859700	3.28456900
H	5.83022000	0.12051600	2.41200100

S-TS2

Thermal Correction to Free Energy: 0.336902 Hartree
SCF energy: -1320.992750 Hartree
Gibbs free energy: -1320.655848 Hartree
Coordinates:

C	-0.54728800	1.82078900	1.28576000
C	1.29483500	1.90527300	-0.15924300
C	0.86147100	3.10088000	-0.71540500
C	-0.33548700	3.65356500	-0.26674000
C	-1.02066000	3.02972600	0.76244200
H	1.44316800	3.59698600	-1.47903300
H	-0.70499400	4.57702900	-0.69521000
H	-1.91957600	3.46667500	1.17833800
C	2.61776100	1.29905700	-0.43678400
C	3.63164000	1.92669000	-1.15358000
C	4.88360200	1.32074500	-1.19398200
H	3.46474400	2.87334700	-1.64739500
C	4.03626500	-0.45701400	0.19275100
C	5.09675500	0.14002800	-0.49380600
H	5.69366700	1.78538100	-1.74282700
H	6.07471900	-0.32286900	-0.47120900
N	0.55332000	1.23892700	0.77349100

N	2.81664700	0.10817000	0.17131300
C	-1.21158400	1.20868300	2.48168100
H	-0.76233000	0.25133200	2.72838000
H	-1.08735300	1.88393100	3.33384900
H	-2.28079900	1.07728900	2.31602000
C	4.20025300	-1.71546800	0.99152400
H	3.68846000	-2.53507600	0.48409100
H	5.25351500	-1.96771600	1.11501900
H	3.74237200	-1.59037100	1.97580800
Ni	1.04671100	-0.64393800	0.65797500
C	-1.68351700	-1.39103900	0.24037900
H	-1.52353600	-1.34478400	-0.83260900
C	-0.49770100	-1.73204500	1.01403300
H	-0.65967200	-1.83604300	2.08870400
C	0.49778400	-2.66851000	0.42508600
C	1.35210400	-2.18237200	-1.09832300
O	2.35853300	-2.86233800	-1.25339300
O	0.69663900	-1.42189600	-1.81380600
C	-2.89313500	-1.09834600	0.75940400
H	-3.02380600	-1.19035900	1.83573900
H	0.03564200	-3.44141000	-0.19039500
H	1.17220000	-3.15641300	1.12847500
C	-4.07923000	-0.65296300	0.02605700
C	-5.30105300	-0.52244300	0.71229200
C	-4.06412000	-0.33013100	-1.34577200
C	-6.45774400	-0.10239600	0.06049300
H	-5.33780700	-0.75804000	1.77121700
C	-5.21929500	0.08678900	-1.99617500
H	-3.13863800	-0.39685800	-1.90556800
C	-6.42514800	0.20286900	-1.29941000
H	-7.38506100	-0.01300800	0.61579800
H	-5.17998400	0.32966500	-3.05256400
H	-7.32303300	0.53156200	-1.81005800

S-In1

Thermal Correction to Free Energy: 0.342635 Hartree
SCF energy: -1321.038539 Hartree
Gibbs free energy: -1320.695903 Hartree
Coordinates:

C	0.38967300	-2.58623200	-0.54599400
C	2.37467500	-1.39420600	-0.18433700
C	3.11448300	-2.56656900	-0.10073300
C	2.45409800	-3.78654200	-0.21154100
C	1.09362300	-3.79299400	-0.46987500

H	4.18764700	-2.53612600	0.01908700
H	3.00685000	-4.71514000	-0.14057600
H	0.56148000	-4.72190700	-0.63033700
C	2.99237800	-0.04800100	-0.25092300
C	4.34598300	0.18773600	-0.02709000
C	4.83978600	1.47017200	-0.23921900
H	5.00239100	-0.60332600	0.30587800
C	2.62578200	2.17455200	-0.88137600
C	3.98165300	2.46232300	-0.69260400
H	5.88745700	1.68563000	-0.06803800
H	4.34812600	3.45899300	-0.90169400
N	1.02046600	-1.41495600	-0.33020900
N	2.14689300	0.94272900	-0.62568200
C	-1.06099500	-2.59551100	-0.93897300
H	-1.43847400	-1.58926600	-1.10344900
H	-1.17214900	-3.17129500	-1.86150300
H	-1.67547500	-3.08245100	-0.17792300
C	1.66887000	3.20364300	-1.40513000
H	1.25494100	2.86521700	-2.35973600
H	0.83172500	3.31910000	-0.71624200
H	2.16788100	4.16018600	-1.55982400
Ni	0.24065100	0.33453300	0.05733800
C	-0.30524200	-0.23265300	2.62166200
H	-0.11395700	0.76196800	3.02434500
C	-1.09434800	-0.28287300	1.37084400
H	-1.44995900	-1.29353700	1.17878700
C	-2.24182300	0.74417200	1.29590000
C	-1.61371000	2.11932000	1.04061000
O	-2.15262300	3.17247300	1.35598900
O	-0.45554200	2.04767000	0.43549400
C	0.21404600	-1.28991800	3.26234000
H	0.81698300	-1.17572500	4.15627000
H	0.05844900	-2.30127800	2.89702000
H	-2.79930500	0.79733700	2.23780700
C	-3.22537700	0.37810500	0.19488500
C	-4.37538500	-0.35426900	0.50636100
C	-2.97801400	0.69007100	-1.14797700
C	-5.25221500	-0.77278200	-0.49429100
H	-4.58204900	-0.60410800	1.54205900
C	-3.85366800	0.27692200	-2.15044500
H	-2.08787200	1.25192600	-1.40818400
C	-4.99327100	-0.45998700	-1.82825000
H	-6.13735900	-1.34153200	-0.23109800
H	-3.64389400	0.52952900	-3.18410400

H	-5.67386200	-0.78355400	-2.60769200

S-In2

Thermal Correction to Free Energy: 0.340738 Hartree

SCF energy: -1321.047341 Hartree

Gibbs free energy: -1320.706604 Hartree

Coordinates:

C	1.08593000	-2.94646000	0.38300700
C	-0.48481200	-1.41428100	1.20715400
C	-1.42465100	-2.41592900	1.41190100
C	-1.09284000	-3.72206800	1.06355900
C	0.17357700	-3.99042700	0.56684100
H	-2.38507000	-2.18970200	1.85178100
H	-1.80837300	-4.52262900	1.20539500
H	0.47285600	-5.00131300	0.32132600
C	-0.67749100	-0.00897100	1.61821800
C	-1.92491900	0.53952900	1.89642600
C	-1.98480100	1.85437500	2.34271500
H	-2.82759500	-0.03396400	1.74014100
C	0.42093300	1.96884100	2.19942700
C	-0.80379800	2.56263200	2.52141900
H	-2.94127100	2.31619500	2.55493600
H	-0.81841100	3.57580500	2.90213100
N	0.72962500	-1.67998900	0.66280700
N	0.46983000	0.71045000	1.71858200
C	2.47736000	-3.22514900	-0.10994000
H	3.09331000	-2.32813500	-0.06890900
H	2.93556600	-4.00315900	0.50542100
H	2.45873800	-3.59057600	-1.14002500
C	1.72065100	2.69094700	2.39484400
H	2.25682200	2.75220200	1.44689500
H	1.55793300	3.68941200	2.80078400
H	2.35379300	2.12851600	3.08735900
Ni	1.66129000	-0.05728900	0.19377400
C	0.32126000	0.19642900	-1.88321900
H	0.30896000	1.28491700	-1.90393600
C	1.64378800	-0.41834500	-1.74262800
H	1.64746400	-1.48080400	-1.98192000
C	2.82739900	0.34736000	-2.31978000
C	3.14090600	1.55777600	-1.44549600
O	3.79057100	2.51949500	-1.83776500
O	2.66649500	1.45528200	-0.22868400
C	-0.85891600	-0.46903200	-1.85562800
H	-0.82181800	-1.55608300	-1.81629600

H	2.68788800	0.66758600	-3.35834000
H	3.72003400	-0.28695500	-2.30195500
C	-2.19092900	0.11043300	-1.71191800
C	-3.28247700	-0.74443400	-1.46348600
C	-2.44660700	1.49651300	-1.74607800
C	-4.56274500	-0.24272900	-1.24473200
H	-3.11245100	-1.81559300	-1.42495900
C	-3.72492900	1.99590700	-1.53090400
H	-1.63577100	2.19055300	-1.93399300
C	-4.79369000	1.13201800	-1.27493200
H	-5.38085500	-0.92719500	-1.04790200
H	-3.89115800	3.06743800	-1.55882200
H	-5.78862200	1.52652300	-1.10355200

Ni-CO_2

Thermal Correction to Free Energy: 0.182684 Hartree
SCF energy: -933.843409 Hartree
Gibbs free energy: -933.660726 Hartree
Coordinates:

C	-2.65809600	-0.69348800	0.09402700
C	-1.30326000	1.20811700	-0.03952800
C	-2.41250300	2.04648000	-0.12167200
C	-3.68061400	1.47775200	-0.09202900
C	-3.80575900	0.09963100	0.02012500
H	-2.29985600	3.11745400	-0.20605200
H	-4.56054800	2.10629000	-0.15379600
H	-4.78090400	-0.36869400	0.05020700
C	0.09531600	1.69253400	-0.03715400
C	0.42614500	3.04259800	-0.09279900
C	1.76440100	3.41111200	-0.05416600
H	-0.34357500	3.79723700	-0.16065300
C	2.35262000	1.07751500	0.10616000
C	2.72962400	2.42176500	0.05352300
H	2.04633700	4.45584300	-0.09846100
H	3.78013800	2.67631100	0.10012400
N	-1.43394600	-0.13310800	0.06061200
N	1.04817700	0.72349500	0.04463500
C	-2.73239100	-2.18633100	0.21234800
H	-2.22839100	-2.65727600	-0.63387100
H	-2.20161800	-2.51994600	1.10667800
H	-3.76652200	-2.52661300	0.25623800
C	3.38342900	0.00018400	0.24518300
H	3.17260900	-0.61059000	1.12480800
H	3.35431700	-0.68304900	-0.60367100

H	4.38056200	0.43134000	0.33341800
Ni	0.35083700	-1.07299200	0.00979500
C	1.46943700	-2.50610400	-0.15322600
O	2.55858700	-3.03306000	-0.27499200
O	0.26070000	-2.94916800	-0.09634900

S-TS1'

Thermal Correction to Free Energy: 0.337981 Hartree
SCF energy: -1320.983054 Hartree
Gibbs free energy: -1320.645073 Hartree
Coordinates:

C	-1.19422800	1.95929100	1.33573800
C	0.75285100	2.16961400	0.06339000
C	0.34351100	3.39646300	-0.44682500
C	-0.88257200	3.91357900	-0.03947100
C	-1.64488000	3.19948300	0.87154400
H	0.95863700	3.93414000	-1.15449800
H	-1.23012800	4.86414100	-0.42508800
H	-2.59210500	3.58552600	1.22549100
C	2.06266400	1.56045300	-0.24836700
C	3.13532100	2.26243600	-0.78480400
C	4.35931600	1.61361000	-0.91939300
H	3.03054200	3.30043200	-1.06631500
C	3.38529600	-0.34887200	0.08883200
C	4.48991700	0.31363800	-0.45533500
H	5.20861000	2.13436000	-1.34422100
H	5.44364600	-0.19731400	-0.49118800
N	-0.02128200	1.44554900	0.91725100
N	2.18225700	0.25776900	0.11781500
C	-2.00810600	1.15082700	2.29655000
H	-2.68113400	1.78868300	2.87072200
H	-2.60260000	0.40962400	1.75753700
H	-1.35853600	0.59836800	2.97597700
C	3.54199900	-1.70015100	0.72308400
H	2.58848600	-2.07974700	1.08427000
H	3.96739000	-2.41843700	0.02215700
H	4.22820700	-1.60830400	1.57059900
Ni	0.50345800	-0.53022000	0.57697900
C	1.11453600	-2.94516800	-0.99976100
H	1.00538600	-3.66023800	-0.18729700
C	1.99067100	-3.19396100	-1.98159400
H	2.13183400	-2.49736100	-2.80301400
C	0.28386600	-1.74497200	-0.90421000
H	0.35091900	-1.11500900	-1.79334500

C	-1.06373400	-1.97709300	1.50454100
O	-2.18916000	-1.92974700	1.97277000
O	0.05077000	-2.27829600	1.97809100
C	-1.07573000	-1.88328500	-0.30723500
H	-1.36860400	-2.93633300	-0.30493700
H	2.59977200	-4.09071900	-1.98624900
C	-2.20556900	-1.04704300	-0.83320800
C	-2.00945700	0.20373500	-1.43525200
C	-3.52235500	-1.51178100	-0.70454000
C	-3.08633100	0.96474400	-1.88415700
H	-1.00792700	0.59943000	-1.54676300
C	-4.60190600	-0.75367300	-1.15081800
H	-3.69639300	-2.47095500	-0.23213800
C	-4.39005400	0.49245200	-1.74150500
H	-2.90304500	1.93211700	-2.33844400
H	-5.61037600	-1.13646300	-1.03694200
H	-5.22927600	1.08538100	-2.08730000

S-TS2'

Thermal Correction to Free Energy: 0.337319 Hartree

SCF energy: -1320.989297 Hartree

Gibbs free energy: -1320.651978 Hartree

Coordinates:

C	4.11702400	-0.11754100	0.16762500
C	2.53694700	1.60294700	0.20764100
C	3.40780000	2.44821700	0.88919200
C	4.67430000	1.97908000	1.21864300
C	5.03590100	0.69329800	0.84018100
H	3.10481700	3.44800900	1.16644300
H	5.37096700	2.61354200	1.75269400
H	6.02544700	0.31034600	1.05459100
C	1.19518200	2.02552100	-0.24752800
C	0.77687400	3.34992900	-0.30978500
C	-0.47148400	3.63296200	-0.85626200
H	1.41566000	4.14872100	0.03866200
C	-0.76704100	1.28254400	-1.30340400
C	-1.23420300	2.59790300	-1.37613800
H	-0.82546500	4.65538500	-0.90522000
H	-2.18654500	2.79184800	-1.85281400
N	2.87548400	0.32637000	-0.11742400
N	0.40183200	1.01560900	-0.68735900
C	4.47436800	-1.50338800	-0.27488800
H	5.54700500	-1.67828500	-0.18805900
H	3.94266400	-2.25349000	0.31387200

H	4.16766400	-1.65532400	-1.31208100
C	-1.51283000	0.16893100	-1.97988400
H	-1.07526300	-0.80047600	-1.75017300
H	-2.56603700	0.17069100	-1.69595000
H	-1.45858900	0.32307300	-3.06243000
Ni	1.08346200	-0.71397800	-0.24161700
C	-1.54656500	-1.23531500	0.87912700
H	-1.85084200	-2.08270300	0.27027800
C	-2.44591300	-0.28736000	1.22415000
H	-2.09112000	0.54503600	1.82923400
C	-0.13778800	-1.16072100	1.20189100
H	0.11351100	-0.41091600	1.95450000
C	-3.85285200	-0.22072000	0.83953500
C	-4.64275100	0.84307700	1.31643100
C	-4.46923000	-1.15902500	-0.01339400
C	-5.98470600	0.96276800	0.96730900
H	-4.19024800	1.58302900	1.96878100
C	-5.80975400	-1.03918100	-0.36035500
H	-3.89488700	-1.98700900	-0.41153400
C	-6.57802600	0.02114800	0.12691700
H	-6.56766900	1.79293100	1.35085700
H	-6.25929500	-1.77522400	-1.01791800
H	-7.62263400	0.11165400	-0.14773600
C	1.33385800	-2.94183600	-0.42919300
O	2.24957100	-3.73596600	-0.25618500
O	0.61928400	-2.65566000	-1.41015200
C	0.72570100	-2.35498700	1.15278600
H	1.56406900	-2.36695000	1.84358500
H	0.15893700	-3.28285300	1.24626800

S-In1’

Thermal Correction to Free Energy: 0.342594 Hartree
SCF energy: -1321.035359 Hartree
Gibbs free energy: -1320.692765 Hartree
Coordinates:

C	2.43983900	2.32937400	-0.07166100
C	2.42787700	0.11540200	-0.83143100
C	3.30537100	0.41487800	-1.86868200
C	3.75414400	1.72541400	-1.99921900
C	3.34141400	2.68088000	-1.08232700
H	3.64810100	-0.34893800	-2.55134200
H	4.43924400	1.98831600	-2.79591900
H	3.71012300	3.69721000	-1.13576800
C	1.98804600	-1.25756900	-0.49153600

C	2.40349800	-2.38171000	-1.19277300
C	2.06600900	-3.64183900	-0.70833200
H	2.99317400	-2.28457100	-2.09255600
C	0.97217300	-2.57309400	1.15510800
C	1.38310800	-3.73493600	0.49172900
H	2.36929500	-4.53297200	-1.24368400
H	1.16327800	-4.69742700	0.93570400
N	1.97829500	1.07023400	0.01578200
N	1.20948000	-1.35605300	0.62676900
C	1.97992400	3.33458800	0.94258200
H	2.75276200	4.08575300	1.11251300
H	1.07075300	3.82753800	0.59566700
H	1.73334600	2.83876700	1.88140500
C	0.30787900	-2.67586900	2.49373200
H	0.24341000	-1.70386100	2.97369100
H	-0.69915100	-3.08986500	2.40481300
H	0.88255300	-3.35417000	3.12909100
Ni	0.25958200	0.38392700	0.90673200
C	-1.69213700	0.24890000	2.89476600
H	-1.60913800	1.32688700	3.03164800
C	-1.92496900	-0.50014500	3.98040500
H	-2.03455600	-1.57812000	3.91995800
C	-1.53814000	-0.21477600	1.49360000
H	-1.69557000	-1.29175400	1.40975300
C	-1.91051000	1.98067600	0.40970800
O	-2.59524400	2.95020600	0.10571200
O	-0.62684400	2.03697300	0.63480900
C	-2.48435200	0.55781100	0.55297400
H	-3.48337000	0.65842500	0.99478500
H	-2.01268600	-0.05461800	4.96558000
C	-2.67199400	-0.03349900	-0.83866800
C	-1.83990800	-1.02692700	-1.36533500
C	-3.71136500	0.45511700	-1.64384600
C	-2.03811000	-1.51732600	-2.65752200
H	-1.02907200	-1.42318800	-0.76958100
C	-3.91165200	-0.03147100	-2.93242500
H	-4.35311600	1.23615900	-1.25213200
C	-3.07342000	-1.02285100	-3.44687200
H	-1.37992700	-2.28878400	-3.04243200
H	-4.72273000	0.36134100	-3.53601800
H	-3.22909100	-1.40497400	-4.44954200

S-In2’

Thermal Correction to Free Energy: 0.340671 Hartree

SCF energy: -1321.042215 Hartree
Gibbs free energy: -1320.701543 Hartree
Coordinates:

C	-4.01136400	0.85693700	0.09907000
C	-1.95851500	1.91812700	-0.25417300
C	-2.55021100	2.92316300	-1.01272100
C	-3.92449000	2.87520700	-1.21942100
C	-4.66128900	1.85180000	-0.63952600
H	-1.95768200	3.72249900	-1.43486900
H	-4.41454800	3.63900900	-1.81084400
H	-5.73738800	1.81392600	-0.74928700
C	-0.53430300	1.92454200	0.14725600
C	0.28878100	3.03987200	0.05971300
C	1.54915500	2.98764000	0.65005900
H	-0.05246200	3.94225000	-0.42695000
C	1.05487100	0.75506500	1.40793800
C	1.91533200	1.85633700	1.35981300
H	2.21616100	3.83860800	0.58852800
H	2.86203300	1.80749800	1.88145300
N	-2.67260300	0.87898600	0.24885800
N	-0.11434800	0.77675500	0.74119000
C	-4.77561700	-0.23880800	0.77995500
H	-5.84258500	-0.16077000	0.57133700
H	-4.39519200	-1.20967400	0.46172200
H	-4.62421900	-0.17154900	1.86158000
C	1.38718900	-0.42489100	2.27161300
H	0.70214900	-1.25175700	2.09463500
H	2.41446600	-0.75322600	2.10501600
H	1.29863000	-0.12512600	3.32069900
Ni	-1.29210800	-0.70096000	0.32969800
C	1.42017900	-1.69813100	-0.48561600
H	1.88273800	-2.36601200	0.23789200
C	2.17540800	-0.74175900	-1.06439400
H	1.68352900	-0.06414300	-1.76047200
C	-0.01712600	-1.87139800	-0.68108800
H	-0.32496600	-1.48020800	-1.66090000
C	3.57584300	-0.43249800	-0.78285300
C	4.14044200	0.73391300	-1.33326700
C	4.39560500	-1.22078400	0.04962400
C	5.45349200	1.10448600	-1.05860600
H	3.52922700	1.36129000	-1.97394600
C	5.70730700	-0.85012000	0.32409500
H	4.00693400	-2.13550500	0.48178300
C	6.24623100	0.31599500	-0.22498100

H	5.85764200	2.01204300	-1.49377100
H	6.31527500	-1.47538800	0.96897700
H	7.26895200	0.60194600	-0.00776100
C	-2.05472400	-3.25719300	-0.33890800
O	-2.77735600	-4.22687600	-0.53966300
O	-2.50714200	-2.08777100	0.03768800
C	-0.54227000	-3.29062000	-0.48183500
H	-0.25902200	-3.98330900	-1.28256900
H	-0.14554600	-3.70981300	0.45118400

S-TS3

Thermal Correction to Free Energy: 0.335227 Hartree
SCF energy: -1321.001756 Hartree
Gibbs free energy: -1320.666529 Hartree
Coordinates:

C	-0.34114200	2.97098800	0.09222900
C	1.15825900	1.47599700	1.08969800
C	2.01598700	2.52004400	1.43757000
C	1.67780400	3.81970400	1.08590500
C	0.48539900	4.04788900	0.40759300
H	2.92223900	2.32000300	1.99216400
H	2.32920800	4.64499700	1.34700600
H	0.19049800	5.04952000	0.12239700
C	1.44544000	0.06326800	1.44338500
C	2.73998800	-0.40270200	1.67317400
C	2.91516000	-1.74657100	1.98396400
H	3.59396800	0.25295500	1.57442800
C	0.53672300	-2.04432300	1.79844100
C	1.80431300	-2.57838600	2.05003900
H	3.90969500	-2.14246900	2.15122300
H	1.91044000	-3.63092400	2.28325000
N	0.00070700	1.70709900	0.42400800
N	0.37099700	-0.74761200	1.50261500
C	-1.64093400	3.15137500	-0.63635500
H	-2.45962900	2.71665800	-0.05697400
H	-1.85336000	4.20476600	-0.82125600
H	-1.60977000	2.61678000	-1.58970400
C	-0.70887600	-2.88595000	1.86507300
H	-1.10166400	-2.90069900	2.88727300
H	-1.47655300	-2.45910500	1.21982700
H	-0.50961400	-3.91805200	1.57027300
Ni	-1.04200400	0.14650100	-0.17376000
C	-1.42401800	-1.23223300	-1.55428500
H	-1.18562600	-2.23022200	-1.19461700

C	-2.79454600	-0.92084200	-1.77123000
H	-2.99769300	-0.02141800	-2.35182100
C	-3.87558500	-1.56465500	-1.20572700
H	-3.74093600	-2.52499400	-0.71501400
H	-4.88050600	-1.31583300	-1.51960500
C	-4.00006800	-0.38367700	0.75052200
O	-5.16070700	-0.32347200	0.95531000
O	-2.86025500	-0.15880200	1.03699000
C	-0.38471800	-0.30792400	-1.93402800
H	-0.66024400	0.47724800	-2.64143400
C	1.05689800	-0.61830100	-1.92861800
C	1.58236200	-1.86646000	-1.55212900
C	1.97233800	0.39881100	-2.26015100
C	2.95619900	-2.08251800	-1.50358900
H	0.91329600	-2.67382600	-1.28140300
C	3.34502100	0.18366900	-2.21042300
H	1.58980500	1.37493700	-2.54160800
C	3.84850700	-1.06184000	-1.82979800
H	3.33220700	-3.05281900	-1.19775500
H	4.02490500	0.98974400	-2.46546700
H	4.91821000	-1.23231500	-1.78553100

S-TS4

Thermal Correction to Free Energy: 0.333662 Hartree
SCF energy: -1320.994755 Hartree
Gibbs free energy: -1320.661093 Hartree
Coordinates:

C	-1.69503600	2.73648100	-0.11083000
C	-3.23306400	0.97724300	-0.21983700
C	-4.27300200	1.86181500	-0.50637700
C	-4.00245300	3.22151300	-0.58570000
C	-2.69967500	3.66292800	-0.38740300
H	-5.27138700	1.48877500	-0.68820100
H	-4.79436900	3.92551100	-0.81094700
H	-2.45391300	4.71519000	-0.44762700
C	-3.44936300	-0.49113600	-0.14317700
C	-4.68172700	-1.05136700	0.19425600
C	-4.78432500	-2.43960800	0.24931400
H	-5.53368300	-0.42824000	0.43106300
C	-2.46006300	-2.58231300	-0.35026600
C	-3.66680500	-3.21595100	-0.02867700
H	-5.72586300	-2.90603000	0.51400300
H	-3.71797300	-4.29770200	0.00321100
N	-1.96669500	1.41603800	-0.02157600

N	-2.36713800	-1.24841200	-0.40231700
C	-0.26799100	3.15310600	0.09892000
H	0.37653100	2.66643500	-0.63803400
H	-0.15080900	4.23380400	0.01497800
H	0.07583200	2.82762100	1.08449200
C	-1.20888900	-3.36586800	-0.64358400
H	-0.87998700	-3.91221100	0.24563800
H	-1.38294700	-4.10269800	-1.43221100
H	-0.41393700	-2.68678300	-0.94969300
Ni	-0.52955300	0.11065700	0.41185800
C	1.77878100	-0.36981900	1.30706700
H	1.95502000	0.63465700	1.68656700
C	0.55749300	-0.96653700	1.68830800
H	0.42327400	-2.03146400	1.50904800
C	-0.48737200	-0.19506900	2.31237500
H	-0.21129800	0.69729500	2.87693700
H	-1.33581200	-0.72932400	2.73684900
C	1.83512100	-0.34589700	-1.56536000
O	2.73991500	-0.37431800	-2.32323600
O	0.66353500	-0.16916400	-1.35264300
C	2.73207600	-0.92058400	0.44338600
H	2.61651900	-1.97868700	0.21271700
C	4.09646300	-0.39672900	0.29283500
C	5.10541300	-1.23542400	-0.21386500
C	4.45230600	0.93293700	0.59233100
C	6.40694600	-0.77759600	-0.40133400
H	4.85867100	-2.26222500	-0.46425800
C	5.75281000	1.39008600	0.40717300
H	3.70276600	1.62383500	0.96170900
C	6.74313500	0.53970500	-0.09022600
H	7.16110800	-1.45282300	-0.79184000
H	5.99494300	2.42009000	0.64752200
H	7.75543000	0.89950800	-0.23477800

S-In3

Thermal Correction to Free Energy: 0.341963 Hartree
SCF energy: -1321.052295 Hartree
Gibbs free energy: -1320.710332 Hartree
Coordinates:

C	-1.28416600	2.90213100	-0.13640700
C	0.58022000	1.91527000	0.84338900
C	1.31468500	3.09683900	0.74791500
C	0.70450000	4.21470600	0.18723500
C	-0.61116000	4.12454200	-0.24583100

H	2.34074100	3.14649600	1.08412400
H	1.25163000	5.14524700	0.09519200
H	-1.11898200	4.98301600	-0.66792400
C	1.12737600	0.67562100	1.45198600
C	2.25223700	0.67969300	2.27570500
C	2.68737900	-0.51919100	2.82527300
H	2.76955400	1.60172200	2.49889300
C	0.85880600	-1.63045400	1.72663400
C	1.98301100	-1.68417500	2.55203600
H	3.55970000	-0.54106600	3.46718800
H	2.29339000	-2.63318200	2.96948500
N	-0.68302500	1.82312100	0.38318600
N	0.45310000	-0.46425900	1.18835200
C	-2.70520900	2.74847000	-0.60406300
H	-3.15128000	1.85807000	-0.16255600
H	-3.29956100	3.62520700	-0.33906600
H	-2.74058800	2.64728400	-1.69352900
C	0.06812600	-2.86108300	1.39152500
H	0.39010600	-3.71194300	1.99185500
H	-0.99584100	-2.67627500	1.54604600
H	0.20157800	-3.10988900	0.33594900
Ni	-1.07271300	-0.36261700	-0.11933000
C	-1.03873200	-1.22614900	-1.88055900
H	-0.86340300	-2.29813400	-1.85965800
C	-2.32587600	-0.69907800	-1.61817900
H	-2.58304000	0.27633000	-2.02374100
C	-3.45867300	-1.54333400	-1.09352800
H	-3.27236800	-2.60818000	-1.27177800
H	-4.41864400	-1.30146100	-1.55267300
C	-3.59349000	-1.37869300	0.44184500
O	-4.61676700	-1.73350200	1.01788700
O	-2.54966800	-0.87712400	1.03626900
C	0.02474200	-0.28732400	-1.85850900
H	-0.20218700	0.72352700	-2.19295600
C	1.45940700	-0.60058500	-1.80584800
C	2.37877300	0.46214100	-1.78691600
C	1.96305300	-1.90795900	-1.70050400
C	3.74409000	0.23170900	-1.64854600
H	2.00981800	1.47958800	-1.86062700
C	3.32825800	-2.13911800	-1.56591600
H	1.28657700	-2.75361600	-1.72235900
C	4.22706200	-1.07154400	-1.53255300
H	4.43092900	1.07055800	-1.62700000
H	3.69270600	-3.15710100	-1.48348100

H	5.28956700	-1.25456700	-1.42126100

S-In4

Thermal Correction to Free Energy: 0.340461 Hartree

SCF energy: -1321.039699 Hartree

Gibbs free energy: -1320.699239 Hartree

Coordinates:

C	-1.04111000	2.76531400	-0.20882100
C	-2.85162900	1.31597000	-0.05689000
C	-3.74240400	2.37284200	0.13343200
C	-3.23996600	3.67036800	0.14642700
C	-1.87990600	3.87328800	-0.04253100
H	-4.79894400	2.19635600	0.27882900
H	-3.90652400	4.51143100	0.29501100
H	-1.46262500	4.87246800	-0.06081600
C	-3.29244100	-0.10097800	-0.13918700
C	-4.61819700	-0.45903900	-0.38324100
C	-4.94457700	-1.80524300	-0.48520800
H	-5.37851300	0.29726400	-0.51564500
C	-2.63063900	-2.34437800	-0.11221600
C	-3.94263900	-2.75714500	-0.35051600
H	-5.96715800	-2.10590900	-0.67861900
H	-4.16366700	-3.81348600	-0.43126700
N	-1.52733500	1.51699100	-0.19437900
N	-2.32657600	-1.03597000	-0.00717300
C	0.44004900	2.92789400	-0.40850300
H	0.83979400	2.05887300	-0.92946000
H	0.66340500	3.83123300	-0.97864200
H	0.95022300	3.01220300	0.55609300
C	-1.50915100	-3.32952000	0.04836700
H	-0.67742600	-3.05870600	-0.60486800
H	-1.13469100	-3.30318600	1.07533300
H	-1.83963100	-4.34356000	-0.17664100
Ni	-0.45135500	-0.42830400	0.35632000
C	1.40903000	-0.21889300	0.99236800
H	1.57791000	0.84805100	1.11393100
C	0.60699300	-0.90312700	1.93594700
H	0.72791300	-1.97204300	2.09507000
C	-0.56024900	-0.22997900	2.36529400
H	-0.54495500	0.84506900	2.52953300
H	-1.31521600	-0.77627700	2.92014800
C	1.65633900	-0.98699300	-1.37868100
O	2.32815500	-1.15229700	-2.39043000
O	0.36268900	-0.88381300	-1.35776600

C	2.33035200	-0.94606900	0.03354000
H	2.36789500	-2.00096100	0.33007600
C	3.73781400	-0.39585800	0.02140600
C	4.00672700	0.86323000	-0.53056800
C	4.79159300	-1.10773800	0.60047900
C	5.29255100	1.39562200	-0.50216900
H	3.20452400	1.42426200	-0.99696600
C	6.08330000	-0.57998100	0.62898400
H	4.60046600	-2.08501700	1.03203000
C	6.33750400	0.67488600	0.07938800
H	5.48170500	2.37122600	-0.93638000
H	6.88828900	-1.14972500	1.08005900
H	7.33973100	1.08784000	0.10006500

T-d1-CO_2

Thermal Correction to Free Energy: 0.331305 Hartree
SCF energy: -1321.012351 Hartree
Gibbs free energy: -1320.681045 Hartree
Coordinates:

C	-0.76995700	2.75399400	-0.32668300
C	-2.46318100	1.13866200	-0.26598100
C	-3.45116700	2.12360600	-0.27761200
C	-3.07088800	3.45778000	-0.32439900
C	-1.71889900	3.77601800	-0.35236800
H	-4.49866800	1.86195700	-0.24734700
H	-3.82118900	4.23884800	-0.33683900
H	-1.39051700	4.80670800	-0.38803100
C	-2.77009900	-0.31034700	-0.23809500
C	-4.07142000	-0.80490500	-0.32179800
C	-4.27096600	-2.17854000	-0.31371700
H	-4.91608600	-0.13679600	-0.40302200
C	-1.88728900	-2.47369900	-0.15033000
C	-3.16970600	-3.01960600	-0.22997700
H	-5.27246800	-2.58569400	-0.37978300
H	-3.29079900	-4.09512900	-0.22812000
N	-1.14873900	1.45971900	-0.28903600
N	-1.70221800	-1.13813800	-0.15109900
C	0.70093100	3.04717200	-0.31569300
H	1.22283400	2.39304700	-1.01623000
H	0.89655500	4.08946700	-0.56732500
H	1.10883700	2.85668800	0.68126400
C	-0.67794500	-3.35677600	-0.04816800
H	0.12633700	-2.96251900	-0.66920900
H	-0.32918100	-3.40471800	0.98747300

H	-0.91507400	-4.37337300	-0.36316400
Ni	0.09392400	-0.13595400	-0.12486800
C	-0.40326800	-0.62021300	2.68272300
H	-0.60013700	-1.68310300	2.57353200
C	0.72908800	-0.09319100	1.94310400
H	0.97202000	0.94805100	2.13975900
C	1.61401500	-0.87379800	1.20133200
C	0.99548600	-0.45111600	-1.97204800
O	0.84416400	-1.60225400	-2.37871100
O	1.54184700	0.57530700	-2.37438300
C	-1.20627300	0.11728600	3.46595900
H	-2.03980900	-0.32603700	3.99667700
H	-1.04866900	1.18413800	3.58966100
H	1.44182800	-1.94618600	1.18463100
C	2.95073400	-0.46701200	0.73111200
C	3.71154200	-1.38279400	-0.01664800
C	3.50929400	0.79556300	0.99104300
C	4.97061600	-1.04578500	-0.50029800
H	3.29634400	-2.36167300	-0.23096100
C	4.76726700	1.13453000	0.50225700
H	2.96302200	1.52013300	1.58201300
C	5.50493800	0.21905000	-0.24907000
H	5.53556500	-1.76941100	-1.07746700
H	5.17569900	2.11651300	0.71408700
H	6.48516600	0.48503500	-0.62746500

T-d2-CO_2

Thermal Correction to Free Energy: 0.333370 Hartree

SCF energy: -1321.018771 Hartree

Gibbs free energy: -1320.685401 Hartree

Coordinates:

C	1.48395600	2.64472700	-0.38074000
C	-0.09645900	1.12061800	-1.19082500
C	-0.90893800	2.15457500	-1.65593900
C	-0.49337700	3.46674400	-1.47907500
C	0.71771700	3.71447100	-0.84407300
H	-1.85576100	1.94513600	-2.13119000
H	-1.10903600	4.28607700	-1.82962100
H	1.07009100	4.72677500	-0.69397100
C	-0.44986700	-0.30811800	-1.34562400
C	-1.52480200	-0.73956000	-2.12106100
C	-1.78438300	-2.10005100	-2.21095500
H	-2.14669500	-0.03295200	-2.65035100
C	0.10116400	-2.50623100	-0.77162300

C	-0.96377000	-2.99118700	-1.53286200
H	-2.61601100	-2.45877400	-2.80487500
H	-1.13937700	-4.05798600	-1.58275700
N	1.07315100	1.37187800	-0.55625000
N	0.34433600	-1.18397400	-0.68759800
C	2.77175200	2.86242400	0.35840200
H	3.51720400	2.12408300	0.06060700
H	3.15540800	3.86926100	0.19319600
H	2.60803800	2.73375800	1.43372200
C	0.98814000	-3.43491500	0.00505200
H	0.91084400	-4.45394600	-0.37531800
H	2.02409000	-3.10099000	-0.05027900
H	0.68620200	-3.44831900	1.05686000
Ni	1.84490300	-0.26632600	0.38874800
C	-0.39221700	-0.32531100	2.08118100
H	-0.60626500	-1.38258400	1.96089500
C	0.97939700	0.01043200	2.36445900
H	1.18699300	1.05266400	2.59911100
C	2.03119600	-0.90222900	2.40080400
H	1.83805500	-1.96944900	2.40340300
H	2.99903200	-0.59427400	2.77795200
C	3.72489000	-0.77741000	-0.29533800
O	3.71480700	-1.76921900	-1.02041000
O	4.56073300	0.02985500	0.11166300
C	-1.35849500	0.59204000	1.83190900
H	-1.09005800	1.64302600	1.91482200
C	-2.70291700	0.32402100	1.33758000
C	-3.49837600	1.40411400	0.90828400
C	-3.23787100	-0.97412400	1.21265000
C	-4.76485300	1.19929800	0.36966800
H	-3.10358000	2.41169300	0.98574000
C	-4.50373800	-1.17653900	0.67869300
H	-2.65817600	-1.83272700	1.52954500
C	-5.27620800	-0.09299700	0.25127100
H	-5.35265800	2.04902300	0.04053600
H	-4.89152800	-2.18539400	0.59050500
H	-6.26247000	-0.25614000	-0.16760900

T-TS1

Thermal Correction to Free Energy: 0.334861 Hartree

SCF energy: -1320.990392 Hartree

Gibbs free energy: -1320.655531 Hartree

Coordinates:

C	1.42858200	2.71958400	0.59070000

C	2.77385700	0.87573400	0.06493100
C	3.81759900	1.70885200	-0.34008300
C	3.65053200	3.08369500	-0.25735000
C	2.44763800	3.59437400	0.22018200
H	4.73865700	1.29646000	-0.72520300
H	4.44741800	3.74973700	-0.56475000
H	2.29087700	4.66203100	0.30261800
C	2.86983900	-0.60127100	0.04426600
C	4.07970100	-1.26723300	-0.14749500
C	4.09269700	-2.65517400	-0.14203500
H	4.99965000	-0.71721100	-0.28188600
C	1.71718700	-2.62630800	0.24864400
C	2.90166000	-3.33995600	0.05654400
H	5.02166100	-3.19378000	-0.28404100
H	2.87717400	-4.42188900	0.06631000
N	1.60155000	1.38273100	0.51192200
N	1.71198100	-1.27786300	0.24632600
C	0.09772800	3.21535000	1.07311300
H	-0.20973300	2.68049400	1.97196100
H	0.12357300	4.28679200	1.26985000
H	-0.66688700	3.01951700	0.31572700
C	0.41404900	-3.34946500	0.42035700
H	-0.26091100	-2.81622300	1.08668400
H	-0.08628400	-3.44535800	-0.54873400
H	0.57982700	-4.35634700	0.80477300
Ni	0.11515300	0.00452800	0.53334500
C	0.23468000	-0.42028300	-2.23787900
H	0.32021500	-1.50518900	-2.21806500
C	-0.74388500	0.15169800	-1.34365400
H	-0.98469000	1.19712900	-1.52004300
C	-1.71766400	-0.65094800	-0.62458700
C	-1.67397800	-0.63521700	1.55156200
O	-2.13844300	-1.66356500	1.98569200
O	-1.44180900	0.51796200	1.96469300
C	1.06153800	0.26937700	-3.05167500
H	1.78097400	-0.23585100	-3.68438100
H	1.03536300	1.35398500	-3.09489600
H	-1.62526700	-1.72319500	-0.76509300
C	-3.13707500	-0.20519500	-0.56063800
C	-4.16064700	-1.16590900	-0.54167400
C	-3.50407800	1.14958400	-0.52382000
C	-5.50004800	-0.78967400	-0.49430200
H	-3.89689500	-2.21768800	-0.55921700
C	-4.84279000	1.52645700	-0.47203800

H	-2.73907300	1.91586200	-0.51651300
C	-5.85003100	0.56040500	-0.45825600
H	-6.27174700	-1.55181600	-0.48655600
H	-5.10115300	2.57945700	-0.44087400
H	-6.89228900	0.85620900	-0.42100600

T-TS2

Thermal Correction to Free Energy: 0.335553 Hartree
SCF energy: -1321.005236 Hartree
Gibbs free energy: -1320.669683 Hartree
Coordinates:

C	0.89989200	2.80662200	-0.70648500
C	-0.44278400	0.97261700	-1.26558100
C	-1.53182000	1.80455600	-1.53186100
C	-1.38119400	3.17412300	-1.38202000
C	-0.15123200	3.68176100	-0.97182700
H	-2.48769700	1.39072600	-1.81637800
H	-2.21447700	3.83913200	-1.57330900
H	-0.00247200	4.74695500	-0.85105300
C	-0.50975800	-0.49824000	-1.39954600
C	-1.56589800	-1.14514100	-2.03768400
C	-1.55490200	-2.53074200	-2.12144800
H	-2.37849100	-0.58194600	-2.47216300
C	0.54571800	-2.53704000	-0.94599500
C	-0.48930600	-3.23242300	-1.57543000
H	-2.36641800	-3.05411100	-2.61199000
H	-0.44872100	-4.31275200	-1.62731000
N	0.74673900	1.47350000	-0.85564100
N	0.52463100	-1.19285100	-0.86237000
C	2.23729100	3.29613600	-0.23488000
H	3.03319500	2.90362400	-0.86992700
H	2.27842800	4.38504500	-0.22839300
H	2.43969200	2.92630700	0.77363900
C	1.68583700	-3.27771400	-0.30963200
H	1.85955800	-4.22727400	-0.81755300
H	2.60213700	-2.69021600	-0.31585400
H	1.44530500	-3.50276400	0.73449300
Ni	1.91104300	0.05543400	0.04212700
C	-0.13751000	-0.26613800	1.89033900
H	-0.25481100	-1.33870700	1.76287700
C	1.20252100	0.19561400	2.03670800
H	1.34176400	1.23681100	2.32081100
C	2.36127900	-0.66211100	2.04037700
H	2.20765900	-1.73484100	2.09093600

H	3.19132900	-0.32379300	2.65156600
C	3.88155000	-0.49309400	0.54002400
O	4.55911600	-1.49481000	0.55850100
O	4.00228000	0.69889900	0.19767200
C	-1.23621900	0.53882400	1.78393000
H	-1.08196800	1.61194600	1.87754500
C	-2.58641400	0.12843600	1.44872200
C	-3.58745500	1.11319600	1.29644800
C	-2.95914700	-1.21297200	1.20478000
C	-4.88407100	0.78031800	0.92013800
H	-3.32888000	2.15334400	1.46680800
C	-4.25531100	-1.54232800	0.83149000
H	-2.22323800	-2.00327000	1.29234300
C	-5.23054900	-0.55126200	0.68424200
H	-5.62714500	1.56267200	0.80774000
H	-4.50800400	-2.58072400	0.64485400
H	-6.23983100	-0.81357500	0.38858600

T-In1

Thermal Correction to Free Energy: 0.337356 Hartree
SCF energy: -1321.044681 Hartree
Gibbs free energy: -1320.707325 Hartree
Coordinates:

C	1.40676400	2.75926700	0.31568200
C	2.72124200	0.99446700	-0.49156600
C	3.45441800	1.86077800	-1.30087600
C	3.14464600	3.21488700	-1.28370300
C	2.11589500	3.67040200	-0.46734900
H	4.24942600	1.49353800	-1.93334800
H	3.70224400	3.90818800	-1.90144300
H	1.85675100	4.72057700	-0.43275700
C	2.96490400	-0.46533200	-0.42266100
C	3.97002200	-1.11225700	-1.14033300
C	4.10550800	-2.48792800	-1.01060300
H	4.63421500	-0.56000700	-1.78895500
C	2.25309100	-2.48675100	0.52132600
C	3.23828500	-3.18426600	-0.17540600
H	4.87910200	-3.01255700	-1.55784000
H	3.31979300	-4.25692800	-0.05827000
N	1.71999200	1.45019400	0.29471000
N	2.13732500	-1.15129900	0.39566100
C	0.26022800	3.18219000	1.18706100
H	0.28028100	2.65212700	2.14002400
H	0.27541900	4.25762700	1.36302100

H	-0.68702400	2.92412400	0.70457600
C	1.26786300	-3.17565300	1.42000400
H	1.50309200	-4.23302500	1.53483800
H	1.25476000	-2.70447700	2.40609200
H	0.25987400	-3.08586200	1.00341700
Ni	0.60136000	-0.03525000	1.12340800
C	-0.41588500	-0.92931400	-1.43357300
H	-0.52375200	-2.00474300	-1.27979500
C	-0.86556000	-0.09423100	-0.33405100
H	-0.97553700	0.95563000	-0.62337400
C	-2.06821000	-0.57528700	0.49028500
C	-2.04450600	0.04371500	1.91356800
O	-3.07731600	0.26494100	2.53739000
O	-0.84949600	0.25320900	2.39258900
C	0.19139400	-0.51784400	-2.56466200
H	0.57497100	-1.22271100	-3.29334300
H	0.33395600	0.53847000	-2.77426700
H	-1.92980000	-1.64969100	0.67380500
C	-3.38473900	-0.39109000	-0.23367600
C	-4.04344500	-1.47842800	-0.81537800
C	-3.93496500	0.88650100	-0.40551200
C	-5.21861400	-1.30102900	-1.54783100
H	-3.63162200	-2.47557300	-0.69488400
C	-5.10658200	1.06956400	-1.13386500
H	-3.44248200	1.74096300	0.04538700
C	-5.75490600	-0.02556100	-1.71055700
H	-5.71347400	-2.15957400	-1.98919500
H	-5.51822000	2.06636100	-1.25140200
H	-6.66786400	0.11628400	-2.27808500

T-In2

Thermal Correction to Free Energy: 0.338354 Hartree
SCF energy: -1321.059947 Hartree
Gibbs free energy: -1320.721594 Hartree
Coordinates:

C	2.56291300	-1.51457700	-0.91488200
C	0.42477400	-1.74316100	0.01867700
C	0.15281600	-2.85237400	-0.78321500
C	1.12448600	-3.28694200	-1.67299700
C	2.34329200	-2.61693600	-1.73843600
H	-0.80141300	-3.35518100	-0.72993900
H	0.93412800	-4.14079800	-2.31173100
H	3.12029100	-2.94057900	-2.41850700
C	-0.53297200	-1.19002300	1.00000700

C	-1.78566300	-1.74661200	1.24954600
C	-2.61119700	-1.14176700	2.18674700
H	-2.12086500	-2.62249700	0.71457200
C	-0.91019000	0.51497700	2.56042700
C	-2.16975000	-0.00538200	2.85485100
H	-3.59323500	-1.55059400	2.38944700
H	-2.79276000	0.48458700	3.59155700
N	1.60922300	-1.09553400	-0.06121700
N	-0.11787300	-0.07700000	1.64752000
C	3.85394900	-0.74931600	-0.92070100
H	4.33444900	-0.82133700	0.05895300
H	4.53850800	-1.12990000	-1.67792200
H	3.66911900	0.31161800	-1.10391800
C	-0.38449300	1.75589500	3.22107300
H	-1.04620100	2.09629800	4.01667100
H	0.60953200	1.57346200	3.63733600
H	-0.28366700	2.55866400	2.48406500
Ni	1.59207300	0.71522300	0.85574300
C	-0.42367600	1.49068300	-0.98020900
H	-1.09008100	2.05919100	-0.33252800
C	0.96711100	1.79916800	-0.85312500
H	1.59347000	1.36086500	-1.63440000
C	1.41901300	3.19070400	-0.44109100
H	0.67261500	3.64036500	0.22655700
H	1.53305900	3.87849200	-1.28685500
C	2.73884500	3.17476200	0.34712900
O	3.49843600	4.13797600	0.33766200
O	2.95718200	2.08417600	1.03690100
C	-0.94672400	0.46846800	-1.71899000
H	-0.26274900	-0.08873600	-2.35612100
C	-2.30863300	-0.03624000	-1.67616600
C	-2.64129800	-1.18708500	-2.42363000
C	-3.32987800	0.52785200	-0.88011000
C	-3.91532100	-1.74462700	-2.37664800
H	-1.87589800	-1.65095100	-3.03770700
C	-4.60245800	-0.02639400	-0.83953400
H	-3.11926000	1.39918500	-0.27152100
C	-4.90969100	-1.16864200	-1.58483000
H	-4.13265600	-2.63332600	-2.95998500
H	-5.36214200	0.43020800	-0.21366700
H	-5.90317700	-1.60042900	-1.54605400

T-TS3

Thermal Correction to Free Energy: 0.331272 Hartree

SCF energy: -1321.003095 Hartree
Gibbs free energy: -1320.671823 Hartree
Coordinates:

C	-2.00995100	-1.80520700	-1.40108900
C	-2.34515100	0.47686400	-1.00304800
C	-3.65638600	0.40007900	-1.47245000
C	-4.14321100	-0.82094000	-1.91635400
C	-3.30975600	-1.93441000	-1.88422300
H	-4.28729200	1.27658100	-1.49879100
H	-5.15768900	-0.90273700	-2.28687800
H	-3.65768200	-2.89957900	-2.22861500
C	-1.71971700	1.73472800	-0.55009900
C	-2.39925300	2.95191900	-0.48751600
C	-1.71380800	4.08515000	-0.07571500
H	-3.44490000	3.01734700	-0.75126200
C	0.26302500	2.73990900	0.18570700
C	-0.36671900	3.97952800	0.26103600
H	-2.22160200	5.04025500	-0.01939000
H	0.19618900	4.84675800	0.58096400
N	-1.54124200	-0.61611000	-0.96783400
N	-0.41019900	1.63972800	-0.21378400
C	-1.07805300	-2.97697000	-1.33206400
H	-1.47883800	-3.83686100	-1.86809000
H	-0.10428800	-2.71506900	-1.75175600
H	-0.92188400	-3.26151100	-0.28886300
C	1.70563400	2.55959700	0.55294500
H	1.78695800	1.96037400	1.46355600
H	2.24177400	2.02060700	-0.23132000
H	2.19713700	3.51660600	0.72645800
Ni	0.28087400	-0.24502000	-0.18387200
C	0.18517600	-1.96529100	2.11164800
H	-0.03528300	-2.90190400	1.60436200
C	1.20027500	-1.16381500	1.54060200
H	1.53422300	-0.31630900	2.13619900
C	1.89773800	-1.47696500	0.33594800
H	1.64133400	-2.41860100	-0.14704700
C	-2.34753100	-0.83807300	2.16640300
O	-2.97023200	-1.79395000	1.81801700
O	-2.20691300	0.34613400	2.20247200
C	-0.60661100	-1.63003100	3.20560700
H	-1.16698500	-2.41027900	3.70704300
H	-0.33977200	-0.76656300	3.80712300
C	3.17694900	-0.90571400	-0.08230400
C	3.69246200	-1.22291700	-1.35963000

C	3.94560700	-0.04086400	0.72594700
C	4.89047900	-0.68686900	-1.81201100
H	3.12525000	-1.89107100	-2.00028200
C	5.14279100	0.49993100	0.26656100
H	3.60751600	0.20468300	1.72538300
C	5.62538400	0.18854700	-1.00534300
H	5.25518800	-0.94860700	-2.79972300
H	5.70808600	1.16408500	0.91201900
H	6.55912300	0.61045800	-1.35864500

T-TS4

Thermal Correction to Free Energy: 0.333107 Hartree

SCF energy: -1321.003092 Hartree

Gibbs free energy: -1320.669985 Hartree

Coordinates:

C	-0.57228600	2.46950100	1.13973200
C	-2.06193700	1.56386400	-0.41926500
C	-2.16390600	2.78453300	-1.08309300
C	-1.45305600	3.87530800	-0.59885400
C	-0.64918900	3.71698100	0.52207200
H	-2.78423700	2.89063200	-1.96087600
H	-1.52226700	4.83523500	-1.09583800
H	-0.07426000	4.54445600	0.91670700
C	-2.79690000	0.34904900	-0.84194700
C	-3.66762000	0.33237200	-1.93076100
C	-4.33932200	-0.84352300	-2.23605400
H	-3.82483900	1.21637800	-2.53110000
C	-3.25485400	-1.89284400	-0.36280700
C	-4.13740100	-1.96469200	-1.44117400
H	-5.01915500	-0.88089300	-3.07851000
H	-4.65723500	-2.89169000	-1.64507800
N	-1.28525400	1.42212000	0.68008100
N	-2.59083600	-0.75340600	-0.08453900
C	0.33023100	2.22470300	2.31056900
H	0.74756500	3.15397400	2.69698100
H	-0.20427500	1.71129500	3.11376600
H	1.15105200	1.57858100	1.98782600
C	-3.01939200	-3.07716100	0.52920300
H	-2.00870000	-3.46754400	0.39090500
H	-3.11568200	-2.78658800	1.57682900
H	-3.72770200	-3.87640500	0.31238900
Ni	-1.19290600	-0.46549000	1.38869200
C	1.52761700	-1.25374500	1.03122800
H	1.91142900	-0.61007700	1.81840600

C	0.36619800	-1.98121500	1.32776900
H	0.03872600	-2.68925100	0.56842700
C	-0.36486300	-1.92193900	2.55353900
H	0.11505400	-1.44768600	3.40936300
H	-1.03311000	-2.73835900	2.80402100
C	1.15652300	0.30876500	-1.12461300
O	1.62079200	1.35102600	-0.74629400
O	0.30193100	-0.19860000	-1.80512900
C	2.18007200	-1.24467400	-0.23054400
H	1.85648400	-2.02326500	-0.91733900
C	3.58763800	-0.84921400	-0.39720900
C	4.32584200	-1.35213700	-1.48551100
C	4.23450300	0.06236800	0.45871700
C	5.64691900	-0.97340300	-1.70431800
H	3.85001500	-2.05240800	-2.16526500
C	5.55618400	0.43996900	0.24045500
H	3.69840100	0.48775500	1.29790500
C	6.27443600	-0.07336900	-0.84100400
H	6.18942700	-1.38341600	-2.54973600
H	6.02900100	1.14328000	0.91814300
H	7.30388300	0.22271700	-1.00785200

T-In3

Thermal Correction to Free Energy: 0.338384 Hartree
SCF energy: -1321.021959 Hartree
Gibbs free energy: -1320.683576 Hartree
Coordinates:

C	-2.08495800	-2.17213100	-1.11824800
C	-2.42049600	0.14266700	-1.00157800
C	-3.76911700	-0.00234200	-1.31718200
C	-4.27309700	-1.27549800	-1.54321100
C	-3.42176100	-2.36973700	-1.45841600
H	-4.42001200	0.85648700	-1.38021200
H	-5.31903400	-1.41121700	-1.78967500
H	-3.78340200	-3.37239100	-1.64468100
C	-1.77200100	1.46228100	-0.81150600
C	-2.44280400	2.66438300	-1.01663700
C	-1.74605300	3.85659300	-0.87267500
H	-3.48821500	2.67833400	-1.28591900
C	0.23062100	2.58561500	-0.36544400
C	-0.39618100	3.81820400	-0.55335000
H	-2.24920900	4.80389200	-1.02350000
H	0.17989700	4.72906200	-0.45516900
N	-1.60896800	-0.93187800	-0.88891600

N	-0.45994700	1.43516200	-0.48112400
C	-1.12979100	-3.32278600	-0.98941100
H	-1.56029900	-4.24143700	-1.38596700
H	-0.19712200	-3.11052900	-1.51834400
H	-0.88224000	-3.48737700	0.06365700
C	1.68908400	2.50474800	-0.02672600
H	1.82239500	2.42668500	1.05541800
H	2.15059000	1.63021300	-0.48424100
H	2.21640200	3.39827400	-0.36130000
Ni	0.18890300	-0.46411000	-0.10601000
C	0.10387200	-0.98698400	2.16020600
H	-0.20253800	-2.01380900	1.97226800
C	1.34352000	-0.55338900	1.70236400
H	1.67824300	0.42436800	2.03624400
C	2.10206400	-1.22660300	0.71042700
H	1.81712000	-2.25621100	0.48477000
C	-2.24612300	-0.16483500	2.38261600
O	-2.80590200	-1.28184800	2.28277400
O	-2.66637800	0.95485000	2.00951300
C	-0.81358400	-0.19294400	3.02603800
H	-0.91149800	-0.67405000	4.00774700
H	-0.43911600	0.82311000	3.16426800
C	3.39740500	-0.81800000	0.18294200
C	3.92953100	-1.50069900	-0.93225600
C	4.16034600	0.23634500	0.72626000
C	5.14799700	-1.13376500	-1.48938400
H	3.36424300	-2.32045900	-1.36404700
C	5.37855300	0.60284800	0.16385200
H	3.80416600	0.76650200	1.60098400
C	5.88077800	-0.07380800	-0.94903000
H	5.52895500	-1.67415000	-2.34909500
H	5.94416600	1.41768900	0.60247800
H	6.83105700	0.21410200	-1.38334100

T-In4

Thermal Correction to Free Energy: 0.339005 Hartree
SCF energy: -1321.015161 Hartree
Gibbs free energy: -1320.676156 Hartree
Coordinates:

C	-1.17686500	2.64612700	0.86638100
C	-2.26336500	1.17488700	-0.59117400
C	-2.68959800	2.22903400	-1.39374400
C	-2.35456100	3.52755800	-1.03164800
C	-1.58646800	3.73928000	0.10369400

H	-3.27484600	2.05053600	-2.28321100
H	-2.68389600	4.36316700	-1.63717000
H	-1.29314500	4.73719400	0.40159900
C	-2.58441800	-0.24222100	-0.88422500
C	-3.26048200	-0.63503900	-2.03591100
C	-3.55899100	-1.97936400	-2.21546300
H	-3.54646000	0.08712500	-2.78571500
C	-2.52039800	-2.44446700	-0.09635700
C	-3.20072200	-2.88914200	-1.23193300
H	-4.07882300	-2.30830100	-3.10695600
H	-3.44339200	-3.93926800	-1.32943400
N	-1.54371700	1.39577500	0.53032100
N	-2.20021900	-1.14363600	0.05025000
C	-0.27196900	2.80859000	2.04733500
H	-0.25548300	3.83907000	2.40140900
H	-0.57233100	2.15725700	2.87112600
H	0.73622600	2.52707700	1.73120300
C	-2.13856100	-3.40855800	0.98944000
H	-1.12281900	-3.78216600	0.83506300
H	-2.17357300	-2.92450500	1.96433900
H	-2.80923700	-4.26812700	0.98988600
Ni	-1.03200500	-0.28432300	1.52528800
C	1.35983400	-0.47901700	1.01355600
H	1.59449600	0.41250300	1.58952400
C	0.71472200	-1.53154800	1.63255100
H	0.58724700	-2.43726700	1.04373600
C	0.02772100	-1.44523900	2.88484600
H	0.38177100	-0.71511400	3.61340200
H	-0.39209800	-2.34675100	3.31225000
C	1.11361700	0.70494400	-1.15783700
O	1.36745900	1.85687100	-0.73463800
O	0.32396200	0.36363400	-2.06561600
C	1.83752400	-0.48777600	-0.40635100
H	1.50579100	-1.41103000	-0.88511700
C	3.35197600	-0.41476900	-0.49748400
C	4.06916700	0.69705800	-0.03203100
C	4.06927500	-1.48451400	-1.04577900
C	5.45891700	0.73414700	-0.11688300
H	3.51742500	1.53869000	0.36466300
C	5.46153900	-1.44852600	-1.13372300
H	3.53159000	-2.35528400	-1.40763700
C	6.16335000	-0.33835300	-0.66749700
H	5.99553400	1.60462300	0.24590000
H	5.99553000	-2.28834300	-1.56542800

H	7.24537600	-0.30759900	-0.73204400

T-TS-iso3

Thermal Correction to Free Energy: 0.339133 Hartree

SCF energy: -1321.020873 Hartree

Gibbs free energy: -1320.681740 Hartree

Coordinates:

C	-2.44375400	-1.68376400	-1.32821400
C	-2.19833000	0.64601500	-1.32023400
C	-3.32349400	0.80368500	-2.12582800
C	-4.01347700	-0.32708500	-2.54492800
C	-3.57468800	-1.57936100	-2.13903400
H	-3.66776000	1.78437000	-2.41802200
H	-4.88996800	-0.22791700	-3.17333600
H	-4.10022800	-2.47668600	-2.43768600
C	-1.42222600	1.79291900	-0.78695200
C	-1.71415500	3.11214300	-1.12611600
C	-0.97541200	4.13621700	-0.54844300
H	-2.50274400	3.34463100	-1.82600300
C	0.28344100	2.47840900	0.65600100
C	0.02451300	3.81728800	0.35794000
H	-1.18494500	5.16889700	-0.79866800
H	0.60802500	4.59150100	0.83807400
N	-1.76810600	-0.58035700	-0.94608200
N	-0.42289700	1.48700800	0.07646400
C	-1.96044400	-3.00712500	-0.81861900
H	-2.54849600	-3.82653000	-1.23067700
H	-0.91232700	-3.16562400	-1.08637800
H	-2.04772200	-3.01198700	0.27272100
C	1.35060900	2.09733200	1.63452200
H	0.92949800	1.45779200	2.41259100
H	2.14231900	1.54300500	1.12733100
H	1.79012200	2.97783100	2.10142600
Ni	-0.12060400	-0.54052100	0.20659800
C	0.24286000	-1.89098700	1.90570200
H	-0.13591900	-2.76038600	1.37148400
C	1.44323200	-1.32017200	1.47458100
H	1.89717400	-0.57882300	2.12225100
C	2.03322900	-1.56646500	0.21528700
H	1.63121700	-2.38177900	-0.38484600
C	-1.93882400	-1.15582500	2.86648000
O	-2.24948100	0.03269600	3.10931400
O	-2.64876400	-2.05975000	2.36114800
C	-0.45698300	-1.56623800	3.18347900

H	-0.49056100	-2.45393800	3.82695900
H	0.05174100	-0.76103400	3.71647200
C	3.22106800	-0.92662500	-0.31465000
C	3.53824900	-1.09225400	-1.68166400
C	4.09336400	-0.13676000	0.46717600
C	4.65123900	-0.48000800	-2.24260200
H	2.88732900	-1.70042000	-2.30122600
C	5.20579100	0.47438800	-0.09935500
H	3.91508400	-0.02009600	1.52931400
C	5.49135500	0.31349300	-1.45703800
H	4.86638100	-0.61969100	-3.29620300
H	5.86067200	1.07282700	0.52426900
H	6.36020300	0.79151000	-1.89403900

T-TS-iso4

Thermal Correction to Free Energy: 0.337614 Hartree

SCF energy: -1321.011471 Hartree

Gibbs free energy: -1320.673857 Hartree

Coordinates:

C	-1.20090000	2.67059800	0.60260700
C	-2.85164300	1.23177500	-0.23427700
C	-3.57771400	2.30424700	-0.74633100
C	-3.09283200	3.59308100	-0.55985800
C	-1.89485500	3.77888500	0.11550400
H	-4.49639400	2.14729300	-1.29153800
H	-3.64202200	4.44167500	-0.94882900
H	-1.48722700	4.77021600	0.26262500
C	-3.26855000	-0.18178600	-0.41253300
C	-4.49215600	-0.52748100	-0.98154300
C	-4.79883600	-1.87042600	-1.15560400
H	-5.19904000	0.23104200	-1.28274500
C	-2.66791600	-2.42827100	-0.18817600
C	-3.87489800	-2.82789200	-0.76541400
H	-5.74474200	-2.16245700	-1.59476900
H	-4.07618700	-3.88232700	-0.90020800
N	-1.69271100	1.42584000	0.43402600
N	-2.38339000	-1.12323300	-0.00336000
C	0.12645900	2.80641600	1.28420600
H	0.39985700	3.85365600	1.40916200
H	0.11001500	2.33285700	2.26996900
H	0.88285900	2.30989200	0.66807100
C	-1.64385200	-3.44162000	0.22418400
H	-0.72476700	-3.29096400	-0.34608200
H	-1.40621000	-3.33486500	1.28340200

H	-2.00185100	-4.45462400	0.04571400
Ni	-0.82089800	-0.28326000	1.07869600
C	1.68785800	-0.62692300	0.93189300
H	1.84941100	0.32710800	1.42786700
C	0.87166000	-1.56308700	1.54339500
H	0.79772200	-2.53283100	1.06207500
C	0.02754300	-1.30427600	2.66493500
H	0.29387700	-0.49495600	3.34459700
H	-0.51319800	-2.12537500	3.11956300
C	1.49347100	0.06107300	-1.43311300
O	1.61579300	1.30265700	-1.34420700
O	0.74708600	-0.60435100	-2.18186400
C	2.34654700	-0.80945100	-0.39594300
H	2.23817900	-1.84840200	-0.71078500
C	3.81697700	-0.44470800	-0.37986800
C	4.25874900	0.83043200	0.00142000
C	4.77525800	-1.39401700	-0.75273700
C	5.61609800	1.14198900	0.00758800
H	3.52603600	1.58163100	0.26355600
C	6.13570600	-1.08343700	-0.75054000
H	4.45313600	-2.38768600	-1.04774900
C	6.56255800	0.18698400	-0.36842100
H	5.93728600	2.13486900	0.30448700
H	6.85976600	-1.83545800	-1.04518300
H	7.61900700	0.43129200	-0.36279900

MECP-1

SCF energy: -1132.358236 Hartree

Coordinates:

C	2.25124400	-2.05005400	-0.76494400
C	2.63031400	0.28645200	-0.48039800
C	3.95477500	0.11288700	-0.98458300
C	4.39587200	-1.12210200	-1.36913200
C	3.52144800	-2.24064900	-1.26850300
H	4.61595400	0.96588700	-1.06071000
H	5.40366100	-1.25045500	-1.74935400
H	3.83850700	-3.22740700	-1.57941600
C	2.09685600	1.53963000	-0.08366000
C	2.81285500	2.77093200	-0.18087200
C	2.23533100	3.94481500	0.21412500
H	3.81989600	2.77540000	-0.57623000
C	0.23533200	2.73206400	0.80986700
C	0.90709300	3.93384200	0.72552900
H	2.78220300	4.87834000	0.13690600

H	0.42395800	4.84754200	1.04583900
N	1.79612000	-0.83375800	-0.36297100
N	0.79020500	1.55203900	0.42500400
C	1.29632700	-3.20438100	-0.64120600
H	1.00794500	-3.34854200	0.40156200
H	0.38176200	-3.00630800	-1.20725900
H	1.74226300	-4.12762800	-1.01242400
C	-1.16967300	2.67766500	1.34029100
H	-1.84346200	2.26597400	0.58640900
H	-1.22602000	2.02501000	2.21572700
H	-1.52426700	3.66918400	1.62306400
Ni	0.00231900	-0.32813100	0.48188500
C	-1.31712500	-1.85580400	1.09726200
H	-1.43102500	-2.59019300	0.30610600
C	-1.99522400	-0.63092900	0.99566300
H	-2.17042000	-0.07923900	1.91606000
C	-0.82263300	-2.35971500	2.37820300
H	-0.70838700	-1.61832100	3.16713200
C	-0.51782100	-3.63818000	2.63304200
H	-0.62507800	-4.40814700	1.87614900
H	-0.15863900	-3.94861500	3.60684900
C	-2.88115400	-0.26517500	-0.12865700
C	-2.74118200	-0.81460200	-1.41577300
C	-3.91425900	0.66188400	0.08474100
C	-3.60132400	-0.44789000	-2.44581800
H	-1.94381600	-1.52089900	-1.61866200
C	-4.77906200	1.02317200	-0.94464300
H	-4.04227000	1.09611000	1.07037700
C	-4.62639000	0.47143500	-2.21588300
H	-3.47058400	-0.87909700	-3.43191600
H	-5.57320200	1.73598900	-0.75244200
H	-5.29775600	0.75334800	-3.01870500

MECP-2

SCF energy: -1132.362123 Hartree

Coordinates:

C	0.71577800	2.61824200	0.35309200
C	2.52829800	1.34567400	-0.46505300
C	3.13742000	2.51746100	-0.96026500
C	2.51962700	3.73650000	-0.79513100
C	1.27526600	3.78589400	-0.13823400
H	4.08546100	2.46013700	-1.47697700
H	2.97704200	4.64307000	-1.17407300
H	0.75123100	4.72435900	-0.01151100

C	3.08328700	0.02471600	-0.65307300
C	4.28530200	-0.22781500	-1.34606000
C	4.71280800	-1.52340800	-1.52856200
H	4.86704700	0.59285400	-1.74217200
C	2.77629000	-2.29394100	-0.31665700
C	3.93996800	-2.58066200	-1.01053900
H	5.63033500	-1.72815000	-2.06726000
H	4.24757700	-3.60983500	-1.14247600
N	1.32674100	1.41048900	0.21764600
N	2.34638100	-1.01884600	-0.13422700
C	-0.60694400	2.64271600	1.05987600
H	-1.27809100	1.89643900	0.63257400
H	-0.47983000	2.39733900	2.11718300
H	-1.07551500	3.62443900	0.98968500
C	1.94333900	-3.39105700	0.28305400
H	2.00504900	-3.35456800	1.37385000
H	0.89079400	-3.27028900	0.01404600
H	2.28371000	-4.37151900	-0.05052600
Ni	0.74071200	-0.40895700	0.86477800
C	-1.97476500	-0.83983400	1.20541100
H	-1.86261400	-1.75738500	0.63162300
C	-3.05427500	-0.04719500	1.00554400
H	-3.15423000	0.83377600	1.63565300
C	-0.90388400	-0.53507500	2.13164300
H	-1.01630000	0.36940600	2.72159200
C	0.10876300	-1.44483400	2.47815700
H	0.02201400	-2.48630200	2.17904500
H	0.71862800	-1.26575900	3.35758500
C	-4.11016000	-0.22329300	0.01410000
C	-5.23965400	0.61701700	0.06196100
C	-4.04658600	-1.17544900	-1.02408400
C	-6.25984200	0.51187700	-0.87853900
H	-5.31095900	1.35953000	0.85074000
C	-5.06591300	-1.27723500	-1.96334100
H	-3.18480900	-1.82782000	-1.10696500
C	-6.17961600	-0.43528300	-1.89923600
H	-7.11694800	1.17322000	-0.81670700
H	-4.98904300	-2.00986900	-2.75926900
H	-6.96937600	-0.51386600	-2.63772700

T-TS5

Thermal Correction to Free Energy: 0.346273 Hartree
SCF energy: -1509.679654 Hartree
Gibbs free energy: -1509.333381 Hartree

Coordinates:

C	-1.34976100	2.77508600	0.62459200
C	-2.78090400	0.92564000	0.80012300
C	-3.40806300	1.46675000	1.91776900
C	-2.98380900	2.70425600	2.38968700
C	-1.95368500	3.36557400	1.73794300
H	-4.20947700	0.94153900	2.41606700
H	-3.45808100	3.14641800	3.25712100
H	-1.60868800	4.33247500	2.08019100
C	-3.16017200	-0.37943200	0.20607000
C	-4.20144800	-1.16965400	0.68604600
C	-4.47181200	-2.37635400	0.05197300
H	-4.79294000	-0.85740800	1.53392500
C	-2.67668400	-1.93247600	-1.48309700
C	-3.70691400	-2.76237200	-1.04152300
H	-5.27581200	-3.00847200	0.40814900
H	-3.90028200	-3.69507600	-1.55445000
N	-1.76907100	1.57686400	0.17923800
N	-2.42226900	-0.76902300	-0.85613800
C	-0.20701100	3.44123300	-0.08531300
H	-0.18556000	3.17501600	-1.14141400
H	-0.26723000	4.52460800	0.02074000
H	0.74235600	3.11628700	0.35203100
C	-1.80407200	-2.29051400	-2.65076700
H	-2.16219500	-3.18749400	-3.15384800
H	-1.77301000	-1.46897100	-3.37137000
H	-0.77858800	-2.46860600	-2.31410200
Ni	-0.86704200	0.46282600	-1.27723500
C	0.32362100	-1.26892200	0.50360600
H	0.41699500	-2.19797100	-0.05839800
C	0.83150800	-0.11266600	-0.09989500
H	0.91553000	0.75484400	0.55427000
C	1.90930500	-0.18957200	-1.17827100
C	1.69797700	0.88643500	-2.27314100
O	2.63258900	1.34024800	-2.91835200
O	0.44888700	1.21406100	-2.47630200
H	1.77507700	-1.13790000	-1.71382200
C	3.29167300	-0.18611600	-0.55778600
C	3.98139400	-1.38543700	-0.35797300
C	3.86287500	1.00033900	-0.08164800
C	5.21209100	-1.40342200	0.29890500
H	3.54885900	-2.31499000	-0.71401300
C	5.09046400	0.98707300	0.57511600
H	3.34643800	1.94065300	-0.23678000

C	5.77080600	-0.21655300	0.76892500
H	5.73200700	-2.34418000	0.44325300
H	5.51838800	1.91617600	0.93562400
H	6.72641700	-0.22739100	1.28092600
C	1.42489500	-1.78807800	2.82344800
O	1.96297900	-0.74177800	3.06605700
O	1.46806700	-2.98005600	2.96856600
C	-0.25599900	-1.35312000	1.77346400
H	-0.88068700	-2.21077700	1.99540000
H	-0.53078800	-0.42876900	2.27210500

T-TS6

Thermal Correction to Free Energy: 0.348022 Hartree
SCF energy: -1509.692765 Hartree
Gibbs free energy: -1509.344743 Hartree
Coordinates:

C	0.53330000	3.03045200	0.84315400
C	-0.82184900	1.90724600	-0.70611400
C	-1.85880000	2.81619900	-0.51240600
C	-1.68235600	3.85069200	0.39625900
C	-0.48019200	3.95787200	1.08293900
H	-2.78919000	2.72022000	-1.05110700
H	-2.47703900	4.56639100	0.56654700
H	-0.31626800	4.75495500	1.79571200
C	-0.91974500	0.75741000	-1.63684900
C	-2.08682500	0.43559500	-2.31990300
C	-2.08386900	-0.66313200	-3.16962000
H	-2.99073500	1.00685000	-2.17702900
C	0.22249800	-1.04658500	-2.60392000
C	-0.92165300	-1.40406700	-3.32036600
H	-2.98468000	-0.93911000	-3.70319800
H	-0.89010900	-2.26257800	-3.97815600
N	0.34730000	2.02718000	-0.03800800
N	0.20483200	0.01630500	-1.77798900
C	1.85652700	3.11049400	1.54564600
H	2.67494900	3.15971500	0.82180600
H	1.90781000	3.98736100	2.18931500
H	2.01585000	2.22041600	2.15892400
C	1.48913300	-1.84423300	-2.70546800
H	1.49681100	-2.44665500	-3.61327000
H	2.36385700	-1.19454600	-2.68732200
H	1.57049400	-2.52403900	-1.85180200
Ni	1.72496800	0.61360100	-0.54315400
C	0.58483600	-1.22284500	1.00276000

H	0.45620400	-2.06104200	0.32147700
C	1.87995100	-0.76546400	1.17593400
H	2.03899200	-0.02931000	1.96318000
C	3.09083800	-1.58774800	0.78823100
C	4.05596200	-0.89031800	-0.18231700
O	5.22671200	-1.23524000	-0.26377400
O	3.52055200	0.04449100	-0.92628000
H	2.77586200	-2.50999400	0.28714500
C	-0.46700900	-1.90505800	3.25573100
O	-1.17950200	-2.86659100	3.11554400
O	0.29440400	-1.36949900	4.02471300
C	-0.58104500	-0.73504600	1.65159800
H	-0.44791400	0.21479500	2.16288100
H	3.65961400	-1.89727400	1.66911700
C	-1.91387200	-0.90106300	1.03686100
C	-2.88547800	0.09797100	1.21014900
C	-2.26957300	-2.03618500	0.28959200
C	-4.14568000	-0.00940200	0.62848900
H	-2.63628600	0.98047000	1.78960000
C	-3.52785300	-2.14499400	-0.29257300
H	-1.55800100	-2.84268000	0.16259400
C	-4.47321500	-1.13014000	-0.13424800
H	-4.86922100	0.78698800	0.76544600
H	-3.77228800	-3.02587900	-0.87627600
H	-5.45070600	-1.21431500	-0.59521300

T-In5

Thermal Correction to Free Energy: 0.349467 Hartree

SCF energy: -1509.690834 Hartree

Gibbs free energy: -1509.341367 Hartree

Coordinates:

C	-1.15706700	2.77749800	0.88132200
C	-2.77363200	1.08601000	0.68609800
C	-3.52046000	1.62460200	1.72691500
C	-3.05918700	2.77521200	2.35776700
C	-1.87784600	3.35818000	1.92888900
H	-4.44417900	1.16489100	2.04463200
H	-3.62442200	3.21284300	3.17108600
H	-1.50207400	4.26046700	2.39266400
C	-3.18960600	-0.12421100	-0.06340700
C	-4.36470200	-0.82151300	0.19868900
C	-4.65605100	-1.95112100	-0.55701800
H	-5.04201500	-0.50102900	0.97601400
C	-2.61724100	-1.61646700	-1.78561500

C	-3.77985800	-2.35209800	-1.55625400
H	-5.56232400	-2.51199400	-0.36556900
H	-3.98529600	-3.22592400	-2.15973600
N	-1.60825000	1.65462700	0.28973900
N	-2.34347600	-0.52956700	-1.03777500
C	0.13208300	3.38277500	0.40899800
H	0.27761400	3.22826300	-0.65866700
H	0.15402700	4.44951300	0.63127000
H	0.97741600	2.92087400	0.92801300
C	-1.63541800	-1.98951300	-2.85656000
H	-1.95542500	-2.88135200	-3.39237700
H	-1.52679700	-1.16846100	-3.57062200
H	-0.65016100	-2.17901000	-2.42266400
Ni	-0.66879200	0.58932200	-1.17200400
C	0.33394000	-1.21770200	0.33228100
H	0.36485900	-2.05782600	-0.35518700
C	1.16070600	-0.16743400	0.10814700
H	1.21111800	0.61986400	0.85676600
C	2.22518600	-0.11871300	-0.96885000
C	2.02403300	1.08562500	-1.92260300
O	2.95808200	1.60930500	-2.50408200
O	0.77600800	1.44317000	-2.08471500
H	2.09506800	-0.99595300	-1.61261200
C	3.59640800	-0.18802800	-0.32350700
C	4.24713500	-1.41849200	-0.19596200
C	4.19487100	0.95168400	0.22549700
C	5.47665700	-1.50988000	0.45523000
H	3.78505700	-2.31175700	-0.60317400
C	5.42158200	0.86285900	0.87891200
H	3.70723400	1.91400200	0.12612300
C	6.06759000	-0.36851700	0.99501200
H	5.97051800	-2.47127200	0.54113400
H	5.87506300	1.75552700	1.29511700
H	7.02351800	-0.43684000	1.50174600
C	0.08744400	-2.65516300	2.38297700
O	-0.02654100	-2.55412700	3.61978600
O	0.55407500	-3.59798000	1.70401700
C	-0.47713100	-1.42599900	1.55632200
H	-1.50371900	-1.70373000	1.30008400
H	-0.50641600	-0.53804100	2.18859300

T-In6

Thermal Correction to Free Energy: 0.350542 Hartree

SCF energy: -1509.697712 Hartree

Gibbs free energy: -1509.347171 Hartree

Coordinates:

C	0.25925600	0.33090400	3.01534200
C	1.27596200	-0.97288800	1.35009900
C	2.48479800	-0.97311000	2.03928600
C	2.57392400	-0.28208300	3.23937000
C	1.45698400	0.38163900	3.72749000
H	3.34845800	-1.48623500	1.64540700
H	3.50870900	-0.25849000	3.78534600
H	1.49900400	0.93074500	4.65842200
C	1.09948800	-1.63856200	0.03806800
C	2.13943000	-2.27811900	-0.62445000
C	1.88785600	-2.87052600	-1.85596300
H	3.13238400	-2.30782000	-0.20393600
C	-0.40388400	-2.15647200	-1.68746200
C	0.61143400	-2.81065500	-2.38970700
H	2.68579500	-3.36897500	-2.39185700
H	0.38590000	-3.26514900	-3.34504000
N	0.18748400	-0.33894100	1.84566000
N	-0.14528500	-1.58277700	-0.49648600
C	-0.97538900	1.01791900	3.51874400
H	-1.82240100	0.32795100	3.53953900
H	-0.82207600	1.41120400	4.52230900
H	-1.23877400	1.85195700	2.86296500
C	-1.79287000	-2.06546900	-2.24583300
H	-1.94057700	-2.79805000	-3.03788100
H	-2.53534700	-2.21874900	-1.46264200
H	-1.96162200	-1.07173800	-2.67137000
Ni	-1.47652400	-0.63268900	0.72055100
C	-1.33206500	1.43882700	-0.77356400
H	-1.37221700	1.00558800	-1.76719800
C	-2.46433200	1.39301600	-0.02912000
H	-2.48426300	1.90687600	0.93042600
C	-3.78542500	0.86802400	-0.52955100
C	-4.25270100	-0.43217800	0.14375900
O	-5.43627500	-0.71766000	0.20957400
O	-3.29134700	-1.20816700	0.58010400
H	-3.72503300	0.65316500	-1.60148900
C	-0.24927000	3.63473600	-1.23081900
O	0.10386200	4.62435500	-0.56919200
O	-0.66813600	3.54878600	-2.40248000
C	-0.11180400	2.22374200	-0.44792200
H	-0.07931000	2.45896800	0.61598600
H	-4.56673600	1.61871800	-0.39657700

C	1.20074600	1.61716800	-0.88201300
C	2.32216600	1.72549800	-0.05330000
C	1.36069600	1.02194800	-2.14184700
C	3.56393300	1.23725100	-0.45718800
H	2.21688200	2.18567100	0.92349300
C	2.59760600	0.52980600	-2.54514900
H	0.51739300	0.95817900	-2.81743900
C	3.70683300	0.63290700	-1.70429800
H	4.41557400	1.32141200	0.20859800
H	2.69515800	0.05899100	-3.51696600
H	4.66849000	0.24297700	-2.01764700

$[Mn(DMA)_5]^{2+}$ (sextet)

Thermal Correction to Free Energy: 0.578304 Hartree

SCF energy: -1543.937903 Hartree

Gibbs free energy: -1543.359600 Hartree

Coordinates:

Mn	-0.49394700	0.01831400	-0.48617300
N	2.96003300	-1.18858100	-2.29925900
C	4.36216600	-0.91164400	-2.61154800
H	4.64709800	-1.46719000	-3.50791300
H	4.52721400	0.14495500	-2.79408200
H	4.99699300	-1.23241100	-1.78223400
C	2.60517500	-2.60589200	-2.18419300
H	1.73000900	-2.71402800	-1.54961500
H	2.39015400	-3.03134100	-3.16802900
H	3.44668900	-3.13958600	-1.74215800
C	2.00903200	-0.25784300	-2.19465200
C	2.37184900	1.20619200	-2.24134300
H	3.16758800	1.44646900	-1.53457400
H	2.70653700	1.48916900	-3.24223100
H	1.48291300	1.78239100	-1.99321500
O	0.80457400	-0.60051000	-2.05146200
N	-2.48767600	-3.07552100	-1.01215300
C	-3.28065300	-4.19534900	-0.49997100
H	-2.60560700	-4.91211300	-0.03066100
H	-3.99619600	-3.86607700	0.24744000
H	-3.81041600	-4.69452000	-1.31594600
C	-1.23879900	-3.45236200	-1.67986200
H	-0.76737600	-2.57703900	-2.11590500
H	-0.55741400	-3.91016300	-0.95845700
H	-1.45689400	-4.18178900	-2.46343300
C	-2.89022500	-1.80053600	-0.97539000
C	-4.22302900	-1.45480300	-0.36260000

H	-5.03237600	-2.07850400	-0.74375800
H	-4.17014900	-1.57662500	0.72223700
H	-4.43233200	-0.41111400	-0.58298400
O	-2.16811600	-0.87561200	-1.43298900
N	-1.59809900	4.16473200	-0.93536100
C	-2.64270700	5.18609900	-0.84095300
H	-2.71687600	5.70316600	-1.79967400
H	-3.60900100	4.74710000	-0.61532100
H	-2.38709300	5.91379500	-0.06691700
C	-0.32503300	4.61623800	-1.50674900
H	0.48430300	3.98164200	-1.15690800
H	-0.36350300	4.58298800	-2.59886000
H	-0.14746900	5.64340400	-1.18826700
C	-1.76373200	2.88448300	-0.60373400
C	-3.04999400	2.42093100	0.03269000
H	-3.37752700	3.09178600	0.82722500
H	-3.84215400	2.36538700	-0.71850500
H	-2.89074900	1.42837400	0.44856000
O	-0.83121200	2.06136900	-0.81939800
N	-0.26229400	-1.58387800	2.84713800
C	0.40149400	-1.73211900	4.14257100
H	1.48001400	-1.79827700	3.98197000
H	0.20239900	-0.88436300	4.78968900
H	0.06143600	-2.64575500	4.63535600
C	0.09107100	-2.58548200	1.83714200
H	-0.73853400	-2.71508100	1.14612000
H	0.97315900	-2.26253700	1.28041500
H	0.29758200	-3.53041400	2.33779400
C	-1.07140400	-0.57378700	2.52335500
C	-1.48797300	0.43193800	3.56775800
H	-1.88329400	-0.04848400	4.46392400
H	-0.63824200	1.05256800	3.86299400
H	-2.25112000	1.07190400	3.13151500
O	-1.50617800	-0.44491500	1.34721000
N	3.24711400	0.56405600	1.73740000
C	4.12683100	1.37244300	2.58084800
C	3.78483800	-0.74607000	1.36354500
C	2.02731100	0.93763400	1.33532400
H	5.03180500	1.63356300	2.02662500
H	3.63972800	2.28441200	2.90873200
H	4.41044100	0.79269800	3.46234000
H	3.17323600	-1.18433100	0.58163300
H	4.80715600	-0.62115300	1.00202600
H	3.79567900	-1.40872100	2.23288400

C	1.49608900	2.30049700	1.70675100
O	1.32865100	0.15839600	0.64108100
H	2.15664000	3.09156400	1.34668400
H	0.51884500	2.42090200	1.24769300
H	1.40133900	2.40491500	2.78945200

D-In5

Thermal Correction to Free Energy: 0.333948 Hartree
SCF energy: -1321.150147 Hartree
Gibbs free energy: -1320.816199 Hartree
Coordinates:

C	1.52174000	2.74884100	0.19906700
C	2.93535000	0.94951600	-0.41131400
C	3.79923800	1.84547100	-1.08028500
C	3.51299600	3.19077300	-1.09004400
C	2.35014600	3.65660400	-0.43472200
H	4.68209300	1.47336400	-1.58355000
H	4.17089800	3.88767600	-1.59642400
H	2.10290600	4.71071100	-0.42379700
C	3.13780200	-0.47172900	-0.32262600
C	4.23073700	-1.16882600	-0.88413300
C	4.32122200	-2.53339700	-0.73718300
H	4.99359400	-0.62936800	-1.43052300
C	2.25403900	-2.50785200	0.50599400
C	3.30680900	-3.22217800	-0.02791200
H	5.15657100	-3.07757300	-1.16217500
H	3.35125200	-4.29623600	0.10202100
N	1.80506200	1.42134900	0.22773500
N	2.16451700	-1.15686400	0.38063800
C	0.25320700	3.17303900	0.88551600
H	0.17183600	2.70078600	1.86671600
H	0.20108600	4.25732600	0.99081900
H	-0.61450400	2.83334700	0.31242800
C	1.13390200	-3.16597500	1.26132200
H	1.28806000	-4.24077300	1.36098800
H	1.03952800	-2.72677000	2.25954100
H	0.18287300	-2.99228700	0.74741500
Ni	0.59307400	-0.04508700	0.85737500
C	-0.69386300	-1.04775200	-1.53338000
H	-0.78486200	-2.10944900	-1.29114000
C	-1.00505800	-0.13866900	-0.44298600
H	-1.13367600	0.89184900	-0.79337500
C	-2.15395100	-0.54287200	0.49523100
C	-1.99853300	0.11814500	1.89289300

O	-2.98380500	0.38634900	2.58249200
O	-0.77283400	0.30382100	2.27242600
C	-0.24939900	-0.73643400	-2.77037900
H	0.03743000	-1.50213800	-3.48283300
H	-0.14056500	0.29818900	-3.08548700
H	-2.03983800	-1.61590200	0.70474700
C	-3.51741300	-0.33489200	-0.12819000
C	-4.24099100	-1.40930700	-0.65581100
C	-4.05023300	0.95381400	-0.27629400
C	-5.45745600	-1.20959100	-1.31176000
H	-3.84530700	-2.41531400	-0.55496500
C	-5.26243900	1.15985900	-0.92788800
H	-3.50813600	1.79924800	0.13266900
C	-5.97387200	0.07681200	-1.45147400
H	-5.99989000	-2.05970100	-1.71216500
H	-5.65686100	2.16578700	-1.02745600
H	-6.91838900	0.23650500	-1.95974100

S-In5

Thermal Correction to Free Energy: 0.332424 Hartree

SCF energy: -1321.198106 Hartree

Gibbs free energy: -1320.865682 Hartree

Coordinates:

C	2.74739800	2.52410500	-0.12769600
C	3.29550800	0.22657300	-0.43412100
C	4.57067200	0.61521600	-0.95372300
C	4.90792000	1.93451000	-1.05886100
C	3.97318100	2.92666600	-0.62134100
H	5.28560000	-0.15394100	-1.22594300
H	5.88185000	2.22828900	-1.43825900
H	4.20582700	3.98242200	-0.69747100
C	2.88359100	-1.09286600	-0.23213900
C	3.53878100	-2.25968900	-0.73468800
C	3.11540300	-3.50899900	-0.38194400
H	4.36980900	-2.14096300	-1.42298000
C	1.34805400	-2.50099600	0.94670700
C	2.01104000	-3.63036600	0.53456900
H	3.60094400	-4.39511200	-0.77795000
H	1.73793000	-4.59552900	0.94667000
N	2.35502000	1.22066700	-0.05987100
N	1.68750600	-1.23723200	0.53183900
C	1.74612900	3.55327600	0.32562800
H	1.48316600	3.40326100	1.37532600
H	2.13383100	4.56539800	0.19085500

H	0.80803600	3.44329500	-0.22307800
C	0.28123100	-2.58693800	2.00943800
H	-0.12654200	-3.59741600	2.09243500
H	0.70919800	-2.30606800	2.97994300
H	-0.52705400	-1.88544700	1.81081900
Ni	0.58059700	0.29762100	0.46934600
C	-1.29058100	-1.70933100	-0.77944100
H	-1.56872000	-2.42910400	-0.00921300
C	-1.13952700	-0.32119200	-0.33655300
H	-1.12004800	0.33849500	-1.21972200
C	-2.22835900	0.18811200	0.62537900
C	-1.79731000	1.57264400	1.16106900
O	-2.62593000	2.37668900	1.60694700
O	-0.52639800	1.78179800	1.12250000
C	-1.10157100	-2.19079400	-2.02000800
H	-1.17873600	-3.25057000	-2.24044300
H	-0.83238500	-1.53532200	-2.84512100
H	-2.23591100	-0.46333100	1.51025300
C	-3.62241600	0.17623000	0.03579300
C	-4.57453500	-0.76504800	0.44026400
C	-3.97172100	1.06267600	-0.99321700
C	-5.83536700	-0.82334500	-0.15727400
H	-4.32422800	-1.46339900	1.23312900
C	-5.22624400	1.01118400	-1.59359500
H	-3.24806400	1.80207900	-1.31945000
C	-6.16704400	0.06470900	-1.17829800
H	-6.55632000	-1.56304100	0.17519700
H	-5.47464200	1.70972000	-2.38597100
H	-7.14470900	0.02292500	-1.64575600

D-In6

Thermal Correction to Free Energy: 0.335249 Hartree
SCF energy: -1321.167498 Hartree
Gibbs free energy: -1320.832249 Hartree
Coordinates:

C	-0.72216400	3.00902800	0.50147100
C	0.66507100	1.22811000	1.19689300
C	1.76889400	2.10276400	1.27202500
C	1.60762500	3.43206100	0.95546500
C	0.33365900	3.89822000	0.56038400
H	2.74186100	1.72389100	1.55252200
H	2.44927300	4.11341700	1.00102200
H	0.17615300	4.93972500	0.30912100
C	0.71605100	-0.18236100	1.49909400

C	1.87446500	-0.86576000	1.91530700
C	1.81181900	-2.21617900	2.17791400
H	2.81192500	-0.33571600	2.01376300
C	-0.52271000	-2.19072600	1.58012100
C	0.58617600	-2.89341900	2.01593800
H	2.69692200	-2.75411200	2.49685100
H	0.50635000	-3.95460800	2.21674400
N	-0.57458400	1.69908100	0.82682800
N	-0.47311800	-0.85684500	1.33713200
C	-2.10187000	3.42384900	0.07379300
H	-2.83826700	3.10750200	0.81912300
H	-2.17613600	4.50287100	-0.06509300
H	-2.36996900	2.93008500	-0.86575200
C	-1.84217300	-2.86193600	1.32512200
H	-1.85214500	-3.88382600	1.70617200
H	-2.65546900	-2.29050100	1.77780600
H	-2.04766700	-2.88480300	0.25073100
Ni	-1.82002800	0.24428500	0.33878900
C	-0.15906700	-0.49224400	-1.71563100
H	-0.05866300	-1.57007200	-1.58784400
C	-1.50054100	-0.01524300	-1.73187600
H	-1.62504300	1.00842000	-2.09633000
C	-2.64203800	-0.94474100	-2.10740100
H	-2.30708100	-1.98720900	-2.02518600
H	-2.98459900	-0.81920300	-3.14177100
C	-3.88154200	-0.84376400	-1.19379400
O	-4.98687600	-1.19882400	-1.61102900
O	-3.65984200	-0.41643800	0.01132000
C	0.98879600	0.26158800	-1.71481500
H	0.87634100	1.33996700	-1.80836600
C	2.34285300	-0.20760200	-1.52746600
C	3.40946500	0.72525100	-1.50791200
C	2.69391500	-1.56653300	-1.33272500
C	4.72822900	0.33021400	-1.31368800
H	3.18013400	1.77838300	-1.63613200
C	4.01357900	-1.95778500	-1.14837500
H	1.91775900	-2.32263600	-1.31190700
C	5.04969500	-1.01819300	-1.13643200
H	5.51331100	1.08023300	-1.30129000
H	4.23827700	-3.00980500	-1.00083100
H	6.07770800	-1.32889300	-0.98803400

S-In6

Thermal Correction to Free Energy: 0.337702 Hartree

SCF energy: -1321.218339 Hartree
Gibbs free energy: -1320.880637 Hartree
Coordinates:

C	1.46397300	2.68937200	-0.42411900
C	-0.38821800	1.40448200	-1.21879600
C	-1.20511000	2.56331400	-1.14243300
C	-0.69406300	3.76222400	-0.72412300
C	0.69847900	3.82718700	-0.38481200
H	-2.25899300	2.47873500	-1.38242200
H	-1.32278900	4.64267000	-0.64706300
H	1.15984400	4.77524000	-0.13114800
C	-0.82718200	0.14686700	-1.69402300
C	-2.06418900	-0.07702400	-2.36899800
C	-2.39557200	-1.33358200	-2.80439800
H	-2.73379300	0.75503100	-2.55140800
C	-0.27226500	-2.13814100	-1.98447700
C	-1.47495800	-2.40097900	-2.62097300
H	-3.33934000	-1.50684400	-3.31212500
H	-1.70634400	-3.40475900	-2.95696600
N	0.96751600	1.46065600	-0.80555000
N	0.04808700	-0.92145900	-1.48618200
C	2.93980600	2.74115700	-0.12470000
H	3.50875900	2.42165600	-1.00629200
H	3.25685900	3.74856100	0.15559000
H	3.20007300	2.04721400	0.67633800
C	0.76032300	-3.22116000	-1.80938100
H	0.33345400	-4.21199000	-1.98070300
H	1.58016400	-3.07588900	-2.52348800
H	1.20776300	-3.16489200	-0.81627100
Ni	1.57165000	-0.20226800	-0.14376300
C	0.23410800	-0.26728100	1.90815000
H	0.13169300	-1.34684500	2.02409400
C	1.59269700	0.21994800	1.81362500
H	1.69023100	1.29025600	2.00231000
C	2.70060800	-0.63056100	2.42100900
H	2.52349500	-0.93263300	3.46262800
H	3.63744000	-0.05930800	2.42384300
C	2.99011700	-1.89436700	1.59318800
O	3.55949600	-2.86634100	2.10922500
O	2.62715900	-1.83174000	0.35572600
C	-0.91354200	0.48314500	1.79430900
H	-0.79479600	1.55690200	1.67358300
C	-2.26293800	-0.00943800	1.68217600
C	-3.34465300	0.90428800	1.57261300

C	-2.60641900	-1.38811100	1.64938600
C	-4.66084800	0.47755500	1.44964400
H	-3.12433000	1.96763700	1.57182000
C	-3.92508600	-1.80830100	1.53195400
H	-1.82172300	-2.13459400	1.70087800
C	-4.97369100	-0.88633900	1.43512900
H	-5.45394900	1.21479400	1.36421700
H	-4.14092800	-2.87260700	1.50728100
H	-6.00065700	-1.22086600	1.34154200

D-TS5

Thermal Correction to Free Energy: 0.340995 Hartree

SCF energy: -1509.793154 Hartree

Gibbs free energy: -1509.452159 Hartree

Coordinates:

C	-1.52632300	2.76871500	0.66836600
C	-2.86851200	0.83239500	0.83884700
C	-3.48759600	1.34614800	1.99502500
C	-3.11516100	2.58410200	2.47239200
C	-2.11566600	3.31178000	1.79597300
H	-4.24600700	0.76990100	2.50783900
H	-3.58398700	2.99352900	3.35947100
H	-1.80818700	4.28914400	2.14604100
C	-3.18091200	-0.44814000	0.24066600
C	-4.17014900	-1.33095100	0.71509000
C	-4.38512900	-2.52696700	0.06602100
H	-4.75656800	-1.07231500	1.58685000
C	-2.64240300	-1.95285300	-1.49848000
C	-3.60056600	-2.84698600	-1.06298800
H	-5.14362700	-3.21559500	0.41885200
H	-3.74465100	-3.78068400	-1.59205100
N	-1.90081900	1.55630100	0.18551000
N	-2.43784300	-0.76319200	-0.87231600
C	-0.44157900	3.47987500	-0.08941700
H	-0.65757300	3.46931200	-1.16020500
H	-0.32509500	4.50884800	0.25187000
H	0.51130400	2.95788500	0.03414400
C	-1.76071900	-2.22891500	-2.68255700
H	-2.02056400	-3.16770100	-3.17183300
H	-1.83693900	-1.41337200	-3.40850800
H	-0.71280700	-2.27470400	-2.36735000
Ni	-0.91010100	0.46528400	-1.16268700
C	0.35796500	-1.26238100	0.52119100
H	0.44704300	-2.17074300	-0.07640600

C	0.81585200	-0.07595500	-0.08418800
H	0.92725200	0.77237900	0.59366200
C	1.87443700	-0.12417000	-1.18206500
C	1.61570000	0.94044200	-2.28498800
O	2.54503700	1.40312000	-2.94642600
O	0.36742400	1.23765900	-2.47273800
H	1.75282600	-1.07886500	-1.71115200
C	3.26727400	-0.08841100	-0.58807700
C	3.97117300	-1.27432900	-0.35393100
C	3.83573800	1.11571500	-0.15155800
C	5.20614200	-1.26305200	0.29545700
H	3.54268100	-2.21849400	-0.67523700
C	5.06747800	1.13282200	0.49736900
H	3.30996300	2.04599200	-0.33316400
C	5.76002600	-0.05840200	0.72467500
H	5.73337000	-2.19553800	0.46660100
H	5.49026500	2.07655400	0.82550900
H	6.71926200	-0.04573900	1.23011100
C	1.82910500	-1.86385500	2.70637300
O	2.21833400	-0.79417400	3.04378800
O	1.94204100	-3.04303000	2.61222000
C	-0.17411100	-1.40480800	1.79348200
H	-0.71406000	-2.30899900	2.04979600
H	-0.40553500	-0.52002100	2.37723000

D-TS6

Thermal Correction to Free Energy: 0.340834 Hartree

SCF energy: -1509.809119 Hartree

Gibbs free energy: -1509.468286 Hartree

Coordinates:

C	0.90436400	3.07820400	0.14425600
C	-0.54585100	1.73285400	-1.13251600
C	-1.56566700	2.69101000	-1.02056600
C	-1.33163400	3.85124300	-0.31030000
C	-0.07377500	4.04945900	0.28237700
H	-2.53080200	2.51430800	-1.47338000
H	-2.10925700	4.59889400	-0.20913200
H	0.14089700	4.95190300	0.84071300
C	-0.68260800	0.47479800	-1.84939700
C	-1.85952800	0.05801100	-2.48800100
C	-1.87834600	-1.15303100	-3.14962600
H	-2.74973300	0.66927600	-2.44626800
C	0.40992100	-1.51021300	-2.48743900
C	-0.72011700	-1.94558800	-3.16023000

H	-2.77988800	-1.49263700	-3.64510100
H	-0.70450500	-2.89916000	-3.67317800
N	0.67715000	1.93904500	-0.55470800
N	0.43492500	-0.31442700	-1.84806400
C	2.27066200	3.22376400	0.75099600
H	3.03862000	3.07724100	-0.01466200
H	2.40633500	4.20343000	1.20931300
H	2.43125800	2.45433900	1.51165000
C	1.65854200	-2.33926600	-2.39836400
H	1.63148100	-3.17931300	-3.09298600
H	2.54047400	-1.72516000	-2.59120100
H	1.77342100	-2.72966000	-1.38225200
Ni	1.82474000	0.32271000	-0.55122400
C	0.32301800	-0.95735000	1.19478600
H	0.18662600	-1.92771000	0.72076400
C	1.64220400	-0.58058000	1.42401500
H	1.79810600	0.29520200	2.05446600
C	2.78322600	-1.57403000	1.39349700
C	3.95665300	-1.19461600	0.46489900
O	5.07913800	-1.65949800	0.67158700
O	3.65778200	-0.41912500	-0.53113400
H	2.41974800	-2.54183300	1.02537000
C	-0.90957100	-0.98609700	3.61719800
O	-1.65413500	-1.91358300	3.61449300
O	-0.17681300	-0.24057100	4.18810100
C	-0.84386000	-0.22815900	1.51277200
H	-0.68952400	0.80473200	1.81212800
H	3.19703600	-1.76263200	2.39017500
C	-2.16610800	-0.51896600	0.96997900
C	-3.16346500	0.48047700	0.98066900
C	-2.53995600	-1.78187700	0.46528300
C	-4.44525000	0.24088600	0.49999000
H	-2.90900000	1.46644400	1.35563500
C	-3.82389700	-2.02211000	-0.01239100
H	-1.81560100	-2.58738300	0.44405700
C	-4.79213300	-1.01631700	-0.00253700
H	-5.17942400	1.04056900	0.51492300
H	-4.07095800	-3.00584600	-0.39943200
H	-5.79128000	-1.20603100	-0.37839900

S-TS5

Thermal Correction to Free Energy: 0.340944 Hartree

SCF energy: -1509.840401 Hartree

Gibbs free energy: -1509.499458 Hartree

Coordinates:

C	-2.92395200	-2.47383600	-0.75040300
C	-3.46941500	-0.17253700	-0.62845100
C	-4.68535600	-0.42743000	-1.32228400
C	-4.99372300	-1.69834600	-1.73319000
C	-4.08899300	-2.75592600	-1.43826600
H	-5.38460000	0.38405400	-1.48834400
H	-5.92491800	-1.90111000	-2.25198000
H	-4.29076800	-3.76837300	-1.76825500
C	-3.09409700	1.09149000	-0.11359900
C	-3.69019200	2.32497300	-0.48731700
C	-3.32424200	3.49527400	0.12259500
H	-4.42560100	2.33342500	-1.28465400
C	-1.75264600	2.24145200	1.48500900
C	-2.34270500	3.43778500	1.16339400
H	-3.76262200	4.44237300	-0.17160400
H	-2.09759600	4.32514900	1.73649400
N	-2.57813200	-1.21591800	-0.35934200
N	-2.05988900	1.05719500	0.84883200
C	-1.92533300	-3.55892900	-0.45033200
H	-1.64516300	-3.54404500	0.60353500
H	-2.31179200	-4.54303700	-0.72332900
H	-0.99660200	-3.37733300	-1.00153700
C	-0.80946100	2.13681600	2.65403800
H	-0.51338700	3.12223900	3.02115600
H	-1.29570000	1.58817500	3.47013300
H	0.08230400	1.56858800	2.39117000
Ni	-0.94463800	-0.47636900	0.73338900
C	1.00493800	1.43652200	-0.13309000
H	1.32821200	2.00859900	0.73645500
C	0.92252000	0.03398100	0.03825400
H	0.86126900	-0.51464300	-0.91046000
C	1.87553100	-0.64415500	1.02620900
C	1.28154700	-1.99229800	1.49992800
O	2.00997100	-2.89070000	1.94082100
O	-0.00199100	-2.06007900	1.42977700
H	1.90700400	-0.02641500	1.93390900
C	3.28444300	-0.73694100	0.47570800
C	4.22912600	0.25328200	0.76734500
C	3.64690200	-1.74667000	-0.42663800
C	5.49419000	0.24228800	0.17877000
H	3.96514800	1.05058500	1.45510300
C	4.90702900	-1.76226900	-1.01899100
H	2.93336200	-2.52898000	-0.65861000

C	5.83902700	-0.76613600	-0.71944700
H	6.20683200	1.02435200	0.41857800
H	5.16521000	-2.55374600	-1.71493000
H	6.82038300	-0.77763600	-1.18076000
C	2.91821400	2.26385300	-1.91784500
O	3.37411900	3.16974900	-1.29941700
O	2.99518500	1.39080000	-2.71843500
C	0.75442900	2.16887800	-1.27783400
H	0.59111400	3.23886000	-1.20649300
H	0.33897900	1.67340000	-2.15025000

S-TS6

Thermal Correction to Free Energy: 0.343142 Hartree

SCF energy: -1509.864394 Hartree

Gibbs free energy: -1509.521252 Hartree

Coordinates:

C	-1.47565800	0.42468700	2.86118800
C	0.46502000	-0.66913900	2.01670400
C	1.26413800	0.06181800	2.92525700
C	0.70043600	0.95935100	3.79642800
C	-0.71886900	1.11514400	3.77488700
H	2.33938900	-0.06794900	2.89992100
H	1.31086700	1.53526100	4.48263300
H	-1.21165600	1.75228600	4.50111200
C	0.98046900	-1.64761900	1.11845300
C	2.28128400	-2.21215000	1.21184700
C	2.68925000	-3.15066000	0.29614300
H	2.94387000	-1.91132800	2.01369200
C	0.51533700	-3.02810700	-0.73925300
C	1.78747400	-3.57939300	-0.70672700
H	3.68544100	-3.57703400	0.35479100
H	2.08055100	-4.31623400	-1.44500200
N	-0.92761900	-0.45217400	1.94380000
N	0.11866600	-2.05989200	0.11721200
C	-2.97814800	0.53017000	2.86299900
H	-3.41861000	-0.46905800	2.96183100
H	-3.33284400	1.15923100	3.68280900
H	-3.34887800	0.93726600	1.92065000
C	-0.50348000	-3.48387200	-1.74952500
H	-0.03397200	-4.02457800	-2.57419700
H	-1.22899400	-4.15396900	-1.27317300
H	-1.07401700	-2.63407700	-2.12589400
Ni	-1.61445900	-0.73687600	0.20958800
C	-0.66800500	1.09960900	-0.92926600

H	-0.58215400	0.67564700	-1.92865200
C	-1.97925800	1.17331000	-0.38497100
H	-2.08276800	1.83667500	0.47238000
C	-3.18602000	1.09900200	-1.30471800
H	-3.19836500	1.87291700	-2.08364200
H	-4.09993400	1.24426300	-0.71545600
C	-3.34525800	-0.27524900	-1.98330100
O	-4.00972100	-0.37688600	-3.02421100
O	-2.77948600	-1.26128300	-1.37484800
C	0.50741800	1.57252500	-0.31616100
H	0.39479200	1.95652300	0.69286100
C	1.85462500	1.19697200	-0.68443900
C	2.94182000	1.56303700	0.14718800
C	2.17960100	0.49356300	-1.86931500
C	4.25416700	1.24709200	-0.17721600
H	2.72927600	2.08580400	1.07469200
C	3.49669300	0.18387600	-2.19392300
H	1.38666800	0.16909900	-2.53261400
C	4.55254300	0.55676200	-1.35849600
H	5.05537100	1.53947600	0.49535100
H	3.70185800	-0.36297600	-3.10976400
H	5.57688500	0.30999100	-1.61432800
C	0.24464600	3.67011900	-1.37225900
O	-0.34217300	4.26713300	-0.53487300
O	0.76983200	3.52967200	-2.42250300

D-In7

Thermal Correction to Free Energy: 0.347163 Hartree

SCF energy: -1509.825146 Hartree

Gibbs free energy: -1509.477982 Hartree

Coordinates:

C	-1.26506700	2.82524100	0.54333600
C	-2.90313800	1.15932800	0.38780000
C	-3.74820600	1.86006000	1.24969700
C	-3.32679200	3.07930900	1.76101100
C	-2.07723800	3.57017600	1.39782300
H	-4.71767800	1.46509200	1.51756400
H	-3.96705300	3.64255200	2.42900200
H	-1.72573300	4.52455000	1.76919200
C	-3.26572100	-0.12978900	-0.23309000
C	-4.50060400	-0.75742600	-0.05093400
C	-4.74835500	-1.95898200	-0.69714300
H	-5.25718500	-0.31643800	0.58231500
C	-2.54736100	-1.84421400	-1.66203500

C	-3.76109300	-2.50603100	-1.51607400
H	-5.69862000	-2.46281000	-0.56984400
H	-3.92813100	-3.43874000	-2.03947400
N	-1.67661700	1.63732300	0.05280900
N	-2.30736800	-0.67536500	-1.02445900
C	0.10028700	3.31491400	0.14987000
H	0.39091600	2.91457900	-0.82100100
H	0.12724200	4.40539700	0.12461900
H	0.84461500	2.98371900	0.88096900
C	-1.43953300	-2.37221200	-2.52505300
H	-1.73069600	-3.28554300	-3.04291300
H	-1.14700800	-1.61962900	-3.26319300
H	-0.55560000	-2.57925300	-1.91473400
Ni	-0.56517000	0.28117400	-0.98298400
C	0.40030900	-1.11047700	0.63569800
H	0.42291900	-2.07735900	0.14058600
C	1.26784800	-0.14264800	0.23605700
H	1.35742900	0.75688000	0.84109300
C	2.30242400	-0.29161400	-0.85902500
C	2.05601300	0.70843900	-2.03676600
O	3.00019900	1.09521000	-2.72241000
O	0.81857300	1.02067400	-2.23554800
H	2.16710800	-1.27955800	-1.31484700
C	3.70212400	-0.20891300	-0.28647500
C	4.49223800	-1.35353200	-0.15318500
C	4.21147200	1.01179900	0.17515200
C	5.76219700	-1.28492600	0.42167500
H	4.10964500	-2.30774800	-0.50088700
C	5.47552600	1.08477700	0.75341700
H	3.61500000	1.91141400	0.07044000
C	6.25764200	-0.06532700	0.87855200
H	6.36160600	-2.18416300	0.51310000
H	5.85388200	2.03900500	1.10373400
H	7.24334800	-0.00904200	1.32668400
C	-0.10672300	-2.18679100	2.89778200
O	-0.31153600	-1.90559100	4.10130500
O	0.29479000	-3.27539500	2.41683700
C	-0.44026700	-1.05152800	1.87185500
H	-1.49785400	-1.18978500	1.61357900
H	-0.35959400	-0.07668300	2.35796900

D-In8

Thermal Correction to Free Energy: 0.349688 Hartree

SCF energy: -1509.836819 Hartree

Gibbs free energy: -1509.487131 Hartree
Coordinates:

C	-0.56148500	-0.37939000	2.85750300
C	-1.59842300	1.03780800	1.31989400
C	-2.78865400	1.01316300	2.04668800
C	-2.85592400	0.25098600	3.20368000
C	-1.73077500	-0.45209400	3.61493000
H	-3.65004400	1.57670600	1.71990500
H	-3.77217500	0.21101400	3.78013800
H	-1.74752500	-1.04953300	4.51739500
C	-1.44523200	1.81114600	0.06506700
C	-2.50735100	2.47364500	-0.54998900
C	-2.27868700	3.14932100	-1.74030500
H	-3.49980700	2.44981600	-0.12504400
C	0.02177100	2.45521200	-1.63330800
C	-1.00301200	3.13671700	-2.29065500
H	-3.08873300	3.66831200	-2.23829100
H	-0.79438100	3.64474800	-3.22358100
N	-0.50846500	0.34516800	1.72310700
N	-0.20400000	1.81784900	-0.46769600
C	0.67817400	-1.11911500	3.27175500
H	1.56091600	-0.48845200	3.15275500
H	0.61107000	-1.44935500	4.30850300
H	0.81634700	-2.00012100	2.64027800
C	1.40653800	2.37021000	-2.20661100
H	1.54582800	3.08500700	-3.01789200
H	2.15195500	2.53263600	-1.42735900
H	1.57600500	1.36312200	-2.60009400
Ni	1.15767600	0.61503800	0.50817500
C	1.48049700	-1.22372800	-0.67345300
H	1.59345900	-0.83838800	-1.68347300
C	2.54445800	-1.10130100	0.18327800
H	2.54256300	-1.66789000	1.11039000
C	3.83711300	-0.40784100	-0.16800800
C	4.00584000	0.99612600	0.46362800
O	5.13525200	1.41569800	0.72543800
O	2.90818600	1.65608100	0.62259800
H	3.89184500	-0.25177200	-1.25182200
C	0.64877400	-3.47672600	-1.44367700
O	0.46302900	-4.59552100	-0.91709900
O	1.00297500	-3.21304200	-2.61628200
C	0.36941700	-2.22736800	-0.50372300
H	0.37255800	-2.60263800	0.52041400
H	4.70040900	-1.01461900	0.11440400

C	-1.01674800	-1.71415200	-0.82430200
C	-2.09144100	-2.02270800	0.01618200
C	-1.27567700	-0.96797800	-1.98194300
C	-3.38284100	-1.58572800	-0.27532700
H	-1.90824300	-2.59286100	0.92087900
C	-2.56298100	-0.52923700	-2.27645600
H	-0.46091100	-0.73375800	-2.65452800
C	-3.62452800	-0.83276700	-1.42268500
H	-4.19585000	-1.82106100	0.40293000
H	-2.73658400	0.06478700	-3.16704200
H	-4.62485300	-0.47883400	-1.64585200

S-In7

Thermal Correction to Free Energy: 0.348972 Hartree
SCF energy: -1509.893748 Hartree
Gibbs free energy: -1509.544776 Hartree
Coordinates:

C	-0.09998600	-2.92960500	-0.39305300
C	-2.31118000	-2.16045200	-0.44287200
C	-2.76591700	-3.40736000	-0.88930300
C	-1.85191500	-4.42895500	-1.09124500
C	-0.50097100	-4.18629800	-0.83461800
H	-3.81884500	-3.58159100	-1.06238500
H	-2.18316100	-5.40252700	-1.43269500
H	0.23873000	-4.96525500	-0.97376700
C	-3.20355600	-1.02385000	-0.17078300
C	-4.56897300	-1.04003800	-0.47198300
C	-5.34969200	0.05884500	-0.15231200
H	-5.01450600	-1.89896600	-0.95457200
C	-3.38440800	1.11368300	0.77453100
C	-4.74802000	1.13656800	0.49822200
H	-6.40788800	0.07128900	-0.38410500
H	-5.33510400	1.99486300	0.80210600
N	-0.99108400	-1.92504000	-0.21085600
N	-2.60164400	0.06443900	0.39943000
C	1.33328600	-2.60558400	-0.10510300
H	1.41159400	-2.11204600	0.86369300
H	1.96429100	-3.49528000	-0.13047600
H	1.70657000	-1.87954400	-0.83172800
C	-2.74403500	2.25134000	1.52147800
H	-3.49047600	2.77846700	2.11964100
H	-1.95659200	1.87530600	2.17481100
H	-2.28008300	2.97117400	0.84145700
Ni	-0.59234600	0.03905100	0.30724300

C	0.03808800	1.82982000	-0.09481400
H	0.06955900	2.47172000	0.79030200
C	1.10445200	0.89894600	-0.25876300
H	1.40301400	0.65719500	-1.27929800
C	2.24863000	0.85317200	0.76187300
C	1.85994500	0.31353700	2.17627300
O	2.71150900	0.46117200	3.08042500
O	0.71628600	-0.21651400	2.31750700
H	2.54856600	1.89165700	0.96793600
C	3.49687200	0.19198700	0.18766700
C	4.06417100	0.73086700	-0.97826600
C	4.11156300	-0.93342900	0.74623800
C	5.18577300	0.15907800	-1.57394200
H	3.61039200	1.61098200	-1.42312000
C	5.23241100	-1.51496000	0.15134800
H	3.71636000	-1.35200300	1.66231700
C	5.77484300	-0.97544300	-1.01332700
H	5.60126200	0.59992400	-2.47413700
H	5.68258700	-2.39302100	0.60299300
H	6.64618900	-1.42697500	-1.47495300
C	-0.19147900	3.97706900	-1.37953600
O	-0.85180800	4.79088100	-0.67375400
O	0.80928000	4.24684800	-2.09504800
C	-0.62909800	2.49730600	-1.29276900
H	-1.71973400	2.45747000	-1.20541400
H	-0.34491100	1.96136600	-2.20414600

S-In8

Thermal Correction to Free Energy: 0.348410 Hartree

SCF energy: -1509.903683 Hartree

Gibbs free energy: -1509.555273 Hartree

Coordinates:

C	-3.29609100	0.10371300	-1.13025600
C	-1.90565500	1.90107800	-0.53321600
C	-2.52995300	2.72949800	-1.47476700
C	-3.55194500	2.22849900	-2.25983200
C	-3.95063100	0.89755900	-2.05679200
H	-2.20416700	3.75516800	-1.59149600
H	-4.04382000	2.84985700	-2.99834600
H	-4.78342800	0.48302300	-2.61314700
C	-0.84413200	2.35099600	0.35280700
C	-0.52498000	3.69987400	0.57518100
C	0.47455800	4.01871100	1.47441400
H	-1.07430000	4.48160700	0.06744800

C	0.79247800	1.66248300	1.88698200
C	1.13706900	2.98196400	2.14501000
H	0.73323200	5.05355400	1.66653300
H	1.92769100	3.19766500	2.85337900
N	-2.23869200	0.56917900	-0.39224500
N	-0.18025700	1.34469700	0.99459400
C	-3.73972300	-1.30952600	-0.87985000
H	-3.64495000	-1.55020400	0.18068800
H	-4.77326600	-1.45760000	-1.19935800
H	-3.10860800	-2.02037400	-1.41785600
C	1.49995000	0.51701100	2.54772200
H	2.13104300	0.86205300	3.36901400
H	0.77454600	-0.21594800	2.90448500
H	2.12271100	0.00870200	1.80731500
Ni	-0.83912600	-0.46585900	0.52677000
C	0.59650100	-1.69036300	-0.07260800
H	1.24641300	-1.98089100	0.75407100
C	-0.68552100	-2.29015300	-0.17431700
H	-1.08269700	-2.43279400	-1.17982800
C	-1.18058100	-3.27278700	0.86571800
H	-0.63496000	-4.22600900	0.84738500
H	-2.23095800	-3.52520900	0.67140700
C	-1.14345600	-2.73582300	2.31547300
O	-1.19064600	-3.55272600	3.25326600
O	-1.10316300	-1.46258000	2.44313500
C	1.34697400	-1.27378700	-1.33353500
H	0.61259500	-0.87097200	-2.03537100
C	2.35994800	-0.18052900	-1.06241700
C	2.04199200	1.15139800	-1.35807400
C	3.60746700	-0.44298700	-0.47893000
C	2.93076200	2.18771000	-1.08087900
H	1.07200800	1.37761200	-1.78819500
C	4.50064800	0.59125200	-0.19927900
H	3.86208700	-1.47330700	-0.26596900
C	4.16781000	1.91317000	-0.49715000
H	2.65109300	3.21115900	-1.30759400
H	5.46056900	0.36387100	0.25386700
H	4.86060000	2.71796200	-0.27555500
C	1.95733300	-2.53878200	-2.03027900
O	1.52904600	-2.78456400	-3.18678000
O	2.78848800	-3.22051500	-1.37407500

D-TS7

Thermal Correction to Free Energy: 0.337695 Hartree

SCF energy: -1509.780358 Hartree
Gibbs free energy: -1509.442663 Hartree
Coordinates:

C	-1.51479900	2.67337300	0.33195400
C	-3.45633000	1.32560800	0.21012000
C	-4.25905700	2.43792300	0.54392500
C	-3.67260700	3.66592100	0.74999300
C	-2.27075400	3.79089600	0.63655300
H	-5.33173900	2.32708900	0.63096200
H	-4.28013200	4.52853700	0.99779500
H	-1.78314200	4.74533400	0.78939200
C	-3.96474100	0.00065300	-0.04662200
C	-5.32613000	-0.36284000	0.03592000
C	-5.70640000	-1.65737600	-0.23652500
H	-6.06875900	0.37324100	0.31405300
C	-3.39702300	-2.21847300	-0.64161800
C	-4.72175000	-2.60790800	-0.58790300
H	-6.74941200	-1.94603300	-0.17984200
H	-4.99246700	-3.63158000	-0.81352000
N	-2.08758200	1.46332300	0.10874300
N	-3.01465600	-0.94094400	-0.38473100
C	-0.01479300	2.72189700	0.25004400
H	0.33468300	2.18605300	-0.63471400
H	0.35293100	3.74832300	0.23288800
H	0.42044100	2.21005200	1.11335700
C	-2.29343100	-3.18003600	-0.98432500
H	-2.68084400	-4.16595600	-1.24131200
H	-1.70375900	-2.79833300	-1.82333100
H	-1.60824600	-3.28005400	-0.13604900
Ni	-1.13780100	-0.27792800	-0.15721900
C	0.73106000	-1.34531500	1.04997900
H	0.69536800	-2.31598300	0.54822500
C	1.84114800	-0.57097700	0.78364300
H	1.89040200	0.41379300	1.24244900
C	2.52751000	-0.71239200	-0.54817600
C	1.61344800	-0.34296900	-1.77982600
O	2.16259500	-0.30451500	-2.88785900
O	0.36149400	-0.13666500	-1.58282700
C	-0.44363000	-0.96017900	1.74045800
H	-0.39957100	-0.06620000	2.36218000
H	2.75900100	-1.77235700	-0.71417200
C	3.32447500	-1.81482400	2.28234700
O	3.60667800	-2.72579600	1.59265900
O	3.30236800	-1.10369400	3.21920400

H	-1.10893400	-1.73608800	2.11300300
C	3.82817400	0.06539300	-0.59607300
C	5.06700200	-0.57922400	-0.54039700
C	3.81143700	1.46603500	-0.63669000
C	6.25727200	0.15014900	-0.53183400
H	5.09693600	-1.66203600	-0.49152900
C	4.99520000	2.19931200	-0.62673100
H	2.85942000	1.98407300	-0.68657000
C	6.22646500	1.54288200	-0.57443300
H	7.20786800	-0.37106600	-0.49092200
H	4.95887100	3.28298200	-0.66210900
H	7.14963000	2.11173500	-0.56829100

D-TS8

Thermal Correction to Free Energy: 0.340105 Hartree
SCF energy: -1509.797767 Hartree
Gibbs free energy: -1509.457662 Hartree
Coordinates:

C	-0.41117800	3.13320600	-0.30581200
C	-1.98401400	1.43561000	-0.67015300
C	-3.03570000	2.31007400	-0.37082500
C	-2.75242300	3.62223000	-0.03460400
C	-1.41852500	4.03964500	-0.00309400
H	-4.06065700	1.96946700	-0.40691400
H	-3.55242500	4.31547300	0.19567300
H	-1.16272400	5.06124900	0.24889400
C	-2.18773200	0.02643400	-1.04364200
C	-3.43321100	-0.60322600	-0.98262600
C	-3.53501100	-1.93775800	-1.33736000
H	-4.30601800	-0.06664300	-0.64010500
C	-1.16468400	-1.95240900	-1.75713800
C	-2.38629400	-2.61950800	-1.73127000
H	-4.49106500	-2.44536400	-1.29349600
H	-2.42758700	-3.66629500	-2.00537800
N	-0.69004900	1.84985200	-0.63758600
N	-1.07068900	-0.64339400	-1.43719400
C	1.03900400	3.51979600	-0.26533300
H	1.56750100	3.11021800	-1.13008900
H	1.16341400	4.60304800	-0.24458600
H	1.51297800	3.10053600	0.62655700
C	0.10558000	-2.67343600	-2.10761300
H	-0.10118300	-3.58551500	-2.66952600
H	0.77827000	-2.02374400	-2.66665800
H	0.63282300	-2.95246100	-1.18908100

Ni	0.64738600	0.34494600	-0.98069200
C	1.55992000	-0.49064100	0.85385100
H	1.56503000	-1.55919200	0.63163700
C	2.73355200	0.20070600	0.51265800
H	2.78858900	1.26529600	0.71402600
C	3.72088800	-0.38186900	-0.45302400
C	3.32601700	-0.43909400	-1.95481400
O	4.21467000	-0.73697600	-2.76684500
O	2.10263300	-0.20646200	-2.27191000
C	0.44762900	0.02046200	1.54842000
H	0.47180700	1.07655400	1.80020000
H	3.94888700	-1.42119900	-0.18058800
C	3.84769700	-0.25288600	2.71376400
O	3.28603800	0.54060500	3.37351800
O	4.58245500	-1.11181500	2.39056800
H	4.68015100	0.14171500	-0.40950500
C	-0.75846200	-0.67240600	1.87782700
C	-1.87619900	0.05719900	2.36973100
C	-0.96067300	-2.06867500	1.68678000
C	-3.09106400	-0.55489900	2.64499500
H	-1.77210500	1.12833100	2.51363600
C	-2.17857400	-2.66971000	1.95917600
H	-0.14781100	-2.67926400	1.31008000
C	-3.26488600	-1.92636200	2.43895000
H	-3.91852600	0.04672400	3.00965000
H	-2.29184300	-3.73585500	1.78659600
H	-4.21544700	-2.40448900	2.64610500

D-In9

Thermal Correction to Free Energy: 0.349247 Hartree

SCF energy: -1509.825742 Hartree

Gibbs free energy: -1509.476495 Hartree

Coordinates:

C	-1.73204700	2.78106700	0.22359300
C	-3.40596200	1.16870500	-0.03426500
C	-4.40300500	2.14429500	0.00160800
C	-4.03232200	3.47551000	0.14629400
C	-2.68486300	3.79991500	0.25276700
H	-5.44692900	1.87997300	-0.08599700
H	-4.78796800	4.25124500	0.17180500
H	-2.36669100	4.82900500	0.36005600
C	-3.68270700	-0.27703600	-0.22336900
C	-4.96942900	-0.78523700	-0.39933500
C	-5.12884900	-2.14757200	-0.61852800

H	-5.83255000	-0.13593200	-0.37605400
C	-2.73994300	-2.40018400	-0.48144600
C	-4.00496700	-2.96091300	-0.67144800
H	-6.11820400	-2.56562800	-0.75922800
H	-4.09564600	-4.02272900	-0.86097400
N	-2.10112700	1.49448500	0.08235800
N	-2.59521400	-1.08320400	-0.24283100
C	-0.26171000	3.05019100	0.36316500
H	0.29348600	2.48885900	-0.39105000
H	-0.03817200	4.11325300	0.27582900
H	0.08829400	2.70050500	1.33948900
C	-1.49945200	-3.24669500	-0.52981300
H	-1.69350700	-4.18826900	-1.04433800
H	-0.68725100	-2.72136800	-1.03508700
H	-1.16438800	-3.48033600	0.48460500
Ni	-0.81925200	-0.09885100	0.16768100
C	0.53058000	-1.10380500	1.38940200
H	0.48445800	-2.17409800	1.20664800
C	1.87285400	-0.47127300	1.10177500
H	1.77642900	0.61599500	1.15456200
C	2.39517000	-0.87957400	-0.29324800
C	1.34656900	-0.78322000	-1.42827700
O	1.41631300	-1.59251500	-2.36023800
O	0.47521300	0.17164700	-1.34916500
C	-0.45070700	-0.50819800	2.16782200
H	-1.26205900	-1.09702500	2.58402600
H	-0.26808100	0.45032600	2.64776300
H	2.68525000	-1.92899700	-0.22795600
C	3.62482700	-0.07174100	-0.66742300
C	4.90031000	-0.64306000	-0.61339200
C	3.51373000	1.27605000	-1.03615200
C	6.03517800	0.10626300	-0.92507500
H	4.99930400	-1.67741600	-0.30473200
C	4.64437600	2.02704400	-1.34922600
H	2.52895800	1.72641000	-1.08483600
C	5.91179500	1.44457800	-1.29580100
H	7.01555700	-0.35568300	-0.87636000
H	4.53729200	3.06784100	-1.63601200
H	6.79263900	2.02832500	-1.53931700
C	2.87230100	-0.90734300	2.23168400
O	3.09983900	-0.05400200	3.12182200
O	3.31649100	-2.08038000	2.15727100

D-In10

Thermal Correction to Free Energy: 0.348661 Hartree
SCF energy: -1509.838894 Hartree
Gibbs free energy: -1509.490233 Hartree
Coordinates:

C	-0.87485600	3.02073500	0.51791800
C	-2.24077600	1.31842000	-0.31801200
C	-3.38562200	1.94159000	0.18223700
C	-3.25139100	3.14388700	0.86283800
C	-1.98409100	3.69164600	1.03296300
H	-4.36254600	1.49789800	0.05625800
H	-4.12521500	3.64623100	1.25988500
H	-1.84818400	4.62683000	1.56125800
C	-2.27541800	0.03311700	-1.05850400
C	-3.46157400	-0.62610600	-1.37918100
C	-3.40047900	-1.80810500	-2.10490400
H	-4.41820400	-0.22726800	-1.07536200
C	-1.00703000	-1.59756500	-2.15243900
C	-2.16307700	-2.29303500	-2.50770400
H	-4.30969000	-2.33810200	-2.36147500
H	-2.08357300	-3.20237000	-3.08939800
N	-1.01504200	1.86087100	-0.15132500
N	-1.07298200	-0.46759700	-1.42489700
C	0.52536600	3.52884900	0.70922100
H	1.11685000	3.36841500	-0.19318800
H	0.53302100	4.58408200	0.98349600
H	1.01485100	2.96249000	1.50874000
C	0.35519700	-2.08800300	-2.55390900
H	0.28946100	-2.79132100	-3.38450400
H	0.99793200	-1.25359100	-2.84135800
H	0.83757500	-2.59819300	-1.71656400
Ni	0.55600000	0.54199700	-0.64422600
C	1.73888500	-0.79452000	0.61122500
H	1.70998800	-1.76649700	0.12665500
C	3.12060300	-0.20866400	0.71495400
H	3.06362000	0.76780100	1.20349700
C	3.81286000	-0.06314000	-0.64813300
C	3.33303400	1.07703900	-1.55895100
O	4.13375700	1.54161600	-2.37863500
O	2.11630500	1.50291600	-1.43647000
C	0.67967900	-0.39104900	1.39834400
H	0.82747500	0.48574700	2.02611000
H	3.70297300	-1.00304700	-1.19987400
C	3.95666800	-1.16299500	1.64299500
O	4.28977200	-0.70106200	2.75930100

O	4.19167500	-2.30541400	1.17580400
H	4.88735600	0.08227600	-0.51183300
C	-0.57952400	-1.11104700	1.63454200
C	-1.61700400	-0.46261400	2.32622400
C	-0.82308000	-2.41183400	1.15847500
C	-2.85266400	-1.07459200	2.51525900
H	-1.45400800	0.54537100	2.69312700
C	-2.05910200	-3.01993600	1.33986800
H	-0.04114200	-2.94832700	0.63513800
C	-3.08480100	-2.35502600	2.01580700
H	-3.63880900	-0.54441300	3.04157700
H	-2.22541200	-4.01845300	0.95084000
H	-4.04903200	-2.83114800	2.15204800

P-1

Thermal Correction to Free Energy: 0.148839 Hartree

SCF energy: -764.697955 Hartree

Gibbs free energy: -764.549115 Hartree

Coordinates:

C	-0.67008400	0.07303600	0.31864000
H	-0.59272500	0.20358400	1.39608200
C	-1.72757300	-0.54710000	-0.20704400
H	-1.80531800	-0.65004800	-1.28786900
C	-2.88966200	-1.09942300	0.56236000
H	-2.80482400	-0.86831000	1.62752900
H	-2.90031900	-2.19626300	0.46934700
C	-4.28286500	-0.62272700	0.03443400
O	-5.15069200	-0.37627700	0.90694000
O	-4.41392800	-0.56152100	-1.21422600
C	0.68736000	2.17808100	-0.14507600
O	0.66493600	2.50096700	1.06948200
O	0.87209800	2.92413900	-1.13431800
C	0.47602400	0.65241000	-0.47079900
H	0.25006300	0.58165200	-1.53748800
C	1.75728600	-0.12368600	-0.20936100
C	2.32831300	-0.91565800	-1.21250400
C	2.38792700	-0.08584900	1.04347700
C	3.49339500	-1.64752900	-0.97788400
H	1.85267600	-0.96161500	-2.18732000
C	3.54901600	-0.81734200	1.28164200
H	1.96185100	0.54696600	1.81228600
C	4.10859300	-1.60363000	0.27223300
H	3.91841100	-2.25251200	-1.77202100
H	4.02180700	-0.77249500	2.25740200

H	5.01269600	-2.17292700	0.45832600

D-In6-Mn

Thermal Correction to Free Energy: 0.818336 Hartree

SCF energy: -2577.193202 Hartree

Gibbs free energy: -2576.374866 Hartree

Coordinates:

C	-2.83765200	-3.03920200	0.70948500
C	-4.22166700	-1.18324700	1.16986600
C	-5.30768900	-2.04062400	1.43392700
C	-5.13912100	-3.40318800	1.32884200
C	-3.88028100	-3.91417000	0.95393400
H	-6.27469200	-1.63034400	1.68908700
H	-5.96764400	-4.07516300	1.51939800
H	-3.72070400	-4.98088900	0.85838600
C	-4.29453300	0.26335100	1.22191300
C	-5.45290900	0.98352300	1.56203600
C	-5.42353500	2.36149600	1.56380400
H	-6.36775900	0.46031200	1.80303100
C	-3.12170600	2.27813800	0.86006300
C	-4.23257000	3.02305600	1.21097300
H	-6.31066600	2.92827000	1.81991300
H	-4.18049000	4.10463000	1.19737700
N	-2.99312600	-1.69522200	0.83052700
N	-3.13597300	0.92041600	0.88154900
C	-1.47196100	-3.52037900	0.30427300
H	-0.74239100	-3.31634900	1.09145400
H	-1.46948900	-4.59148900	0.10077500
H	-1.13200600	-2.98867100	-0.58920500
C	-1.84271400	2.91634900	0.40212400
H	-1.85054400	3.99566500	0.55654300
H	-0.99134100	2.47686300	0.92419700
H	-1.68745700	2.71293500	-0.66177000
Ni	-1.82930600	-0.31277100	0.02856700
C	-3.52604300	-0.03204300	-2.07240600
H	-3.58603500	1.05160600	-2.17210400
C	-2.20250500	-0.56273400	-2.03577700
H	-2.13626600	-1.64506600	-2.16895200
C	-1.04895800	0.19233300	-2.68109100
H	-1.33292700	1.24135900	-2.83852400
H	-0.75290700	-0.20412000	-3.65778200
C	0.17937000	0.24566600	-1.78318500
O	1.33607900	0.17396800	-2.29226800
O	-0.00286200	0.39340900	-0.53503200

C	-4.69133600	-0.72679600	-1.87051200
H	-4.61527700	-1.80685600	-1.76246700
C	-6.02225000	-0.17992600	-1.71904000
C	-7.11776000	-1.05609800	-1.52538000
C	-6.31653400	1.20493800	-1.72522800
C	-8.41523900	-0.58395200	-1.36087000
H	-6.93003200	-2.12495600	-1.49786300
C	-7.61528600	1.67220400	-1.57146900
H	-5.51207900	1.92328300	-1.83160400
C	-8.68250400	0.78710800	-1.38876100
H	-9.22563100	-1.29090900	-1.21186100
H	-7.79774100	2.74240900	-1.57954100
H	-9.69369700	1.15749700	-1.26390900
Mn	2.93241300	0.04741500	-0.92500000
N	2.73699300	3.80040200	-0.75627600
C	2.68583400	5.06628000	-0.02215900
H	1.69342700	5.17206800	0.41771900
H	3.41580200	5.09033700	0.78239500
H	2.85980600	5.91088200	-0.69467400
C	1.50899200	3.43090400	-1.46470400
H	1.73298400	2.69095100	-2.22689100
H	0.78381300	3.00409500	-0.76932700
H	1.08368300	4.32336900	-1.92590900
C	3.83124700	3.03466100	-0.84796300
C	5.10161900	3.48223200	-0.16704700
H	5.36374000	4.51120600	-0.41858800
H	4.99112000	3.41557100	0.91857600
H	5.90276900	2.81616600	-0.47653500
O	3.82294600	1.95156300	-1.48410400
N	6.50004300	-2.06987100	-2.23671400
C	7.94216100	-2.27336700	-2.10481800
H	8.40270900	-2.22179400	-3.09419200
H	8.39823300	-1.51779300	-1.47417000
H	8.14090700	-3.26021700	-1.67838300
C	5.84339400	-2.94948300	-3.20619900
H	4.76697400	-2.82747500	-3.14230100
H	6.17984400	-2.70442300	-4.21708600
H	6.11039300	-3.98576200	-2.98748900
C	5.79791000	-1.15565600	-1.55664300
C	6.49333700	-0.28499400	-0.53804500
H	7.02647000	-0.88690600	0.20000900
H	7.21403200	0.37697400	-1.02335600
H	5.74340700	0.31675700	-0.03294000
O	4.56450600	-1.02832200	-1.76033500

N	2.65495900	1.52712500	2.87530600
C	2.67908000	1.91465500	4.28666100
H	1.83217500	1.46392600	4.81003000
H	3.59822000	1.60386800	4.77142700
H	2.59863500	3.00151000	4.36032900
C	1.53023100	2.06464700	2.10584700
H	1.73252800	3.09657700	1.81095000
H	1.34270800	1.46289200	1.22212600
H	0.64034800	2.04821500	2.73595400
C	3.61236000	0.81244200	2.27160500
C	4.76131500	0.25905200	3.08121900
H	5.39510900	1.06552900	3.45737100
H	4.41179200	-0.32465900	3.93417700
H	5.35530900	-0.37711500	2.43011300
O	3.58450900	0.59336800	1.03930000
N	2.03248500	-2.18152100	2.22956600
C	2.44464900	-2.86914800	3.45268600
C	0.83605800	-1.34744500	2.36484100
C	2.62628700	-2.33661900	1.03732000
H	1.73305400	-3.66240000	3.69812500
H	3.43695600	-3.29792800	3.35665300
H	2.45887900	-2.15002900	4.27421800
H	0.58962800	-0.89807900	1.40822400
H	-0.00186700	-1.95485700	2.71385600
H	1.02338400	-0.56474000	3.10187500
C	3.85605000	-3.20721300	0.92325100
O	2.18526000	-1.75862700	0.01513300
H	3.65453600	-4.23251300	1.23960200
H	4.16746500	-3.20430100	-0.11798500
H	4.67063500	-2.81718700	1.53792400

Int-H

Thermal Correction to Free Energy: 0.259460 Hartree

SCF energy: -1090.030939 Hartree

Gibbs free energy: -1089.771478 Hartree

Coordinates:

C	1.74674200	-2.25425500	-0.52831400
C	2.12310500	0.06448400	-0.22723200
C	3.49127100	-0.18601800	0.02331100
C	3.96923100	-1.47493800	-0.00788100
C	3.07585600	-2.53774500	-0.28873900
H	4.15967000	0.63536900	0.24684800
H	5.01660300	-1.67740500	0.18384300
H	3.42416200	-3.56244400	-0.32371300

C	1.51401200	1.36729600	-0.22762100
C	2.21051100	2.57544500	0.00135400
C	1.53421300	3.77215200	-0.03466300
H	3.27366500	2.55789200	0.20283000
C	-0.50483400	2.56902500	-0.50133100
C	0.14377900	3.77175000	-0.29205900
H	2.05930200	4.70538300	0.13383500
H	-0.41549600	4.69838100	-0.32643000
N	1.26796700	-0.98190500	-0.51317300
N	0.15742700	1.38375600	-0.48787000
C	0.73669600	-3.32588500	-0.82929200
H	0.22567500	-3.10742200	-1.77244200
H	1.19854300	-4.31147000	-0.89550700
H	-0.03239800	-3.34685200	-0.05106200
C	-1.98812800	2.50113000	-0.73352600
H	-2.40159000	3.48470800	-0.96022800
H	-2.21962100	1.80485100	-1.54156900
H	-2.48676300	2.11199300	0.15942800
Ni	-0.64358900	-0.46078000	-0.46956500
C	-0.72821100	-0.01717300	2.32121800
C	-1.41008800	-0.90575900	1.40024500
H	-1.14489000	-1.95872600	1.55409700
C	-2.91121600	-0.71786300	1.20087600
C	-3.38993800	-0.91569000	-0.25032400
O	-4.57302100	-1.17996100	-0.48409700
O	-2.48839300	-0.74360300	-1.16857800
H	-3.19025300	0.31376900	1.45467400
C	0.38871000	-0.25341300	3.04555800
H	0.87639600	-1.22479400	3.02987500
H	-3.53114400	-1.35710000	1.84303500
H	0.85794900	0.52455500	3.63747200
H	-1.14601300	0.99146200	2.37203900

TS1-H

Thermal Correction to Free Energy: 0.264531 Hartree

SCF energy: -1278.673795 Hartree

Gibbs free energy: -1278.409264 Hartree

Coordinates:

C	-1.44524800	1.40760200	-2.17181100
C	-2.25091700	0.09732900	-0.37867500
C	-3.42392300	0.87564700	-0.32172100
C	-3.58973100	1.92443100	-1.19885500
C	-2.57660900	2.19991500	-2.14176000
H	-4.18675000	0.65589100	0.41317600

H	-4.48548900	2.53322400	-1.16450900
H	-2.68068900	3.01682900	-2.84468800
C	-1.96816500	-1.02472800	0.48938000
C	-2.83751700	-1.49319800	1.49394700
C	-2.47116900	-2.57763400	2.26066300
H	-3.78752700	-1.00398700	1.66323000
C	-0.39425600	-2.69647900	1.04085300
C	-1.22247400	-3.19144300	2.03108000
H	-3.13217200	-2.95281700	3.03308900
H	-0.90613200	-4.04313600	2.62023600
N	-1.28136600	0.36398400	-1.31616200
N	-0.76092000	-1.64312500	0.26487900
C	-0.33047000	1.63704800	-3.15305900
H	-0.13833600	0.72300500	-3.72379200
H	-0.56211200	2.44634800	-3.84566900
H	0.59587500	1.87965200	-2.62361900
C	0.96647900	-3.27385200	0.77536900
H	1.11240700	-4.21487900	1.30655900
H	1.11731200	-3.42481700	-0.29552500
H	1.73862600	-2.56745400	1.09563500
Ni	0.40705100	-0.61896600	-0.99554500
C	0.99142500	0.75729900	1.25836800
C	1.69813400	0.71472100	0.03628600
H	1.61293600	1.61387400	-0.57821700
C	3.03754700	0.00814300	-0.06695900
C	3.17035900	-0.95640200	-1.26370800
O	4.28665700	-1.27948200	-1.67486500
O	2.05491500	-1.41228800	-1.74819100
H	3.19981100	-0.61166500	0.82436400
C	1.44713100	3.18150800	2.62061700
O	1.27451100	3.00634300	3.77957000
O	1.92966800	3.71936600	1.68266400
C	0.01594500	1.65810600	1.64672300
H	-0.39059600	2.35640900	0.92176900
H	3.88535200	0.70199400	-0.10661300
H	-0.60256100	1.44256300	2.50917100
H	1.24335000	-0.02558200	1.97578300

TS2-H

Thermal Correction to Free Energy: 0.264749 Hartree

SCF energy: -1278.662064 Hartree

Gibbs free energy: -1278.397315 Hartree

Coordinates:

C	-1.39033400	2.67038800	-0.38030600

C	-2.76603800	0.81161400	0.12845300
C	-3.87018200	1.67168200	0.31239000
C	-3.71959700	3.02770600	0.13107400
C	-2.45230700	3.54065800	-0.23042500
H	-4.83244700	1.26611300	0.59611700
H	-4.56204400	3.69603100	0.26521500
H	-2.30744600	4.60145600	-0.39145200
C	-2.81295400	-0.62170100	0.27829500
C	-3.97876800	-1.35650600	0.58578100
C	-3.91319500	-2.72752000	0.69085300
H	-4.92123800	-0.84526700	0.73047800
C	-1.55082100	-2.62273500	0.22034700
C	-2.67563800	-3.37885100	0.50120700
H	-4.80385600	-3.30216400	0.91732200
H	-2.59574100	-4.45579400	0.57764200
N	-1.53237900	1.32970600	-0.21355400
N	-1.61183800	-1.27413000	0.09760500
C	-0.00920400	3.14143900	-0.74072800
H	0.35968000	2.59797900	-1.61580500
H	0.01138400	4.21091000	-0.95122500
H	0.68649600	2.93065500	0.07661500
C	-0.19132000	-3.24522200	0.05991200
H	-0.25982700	-4.32774700	-0.05378100
H	0.32688900	-2.81346600	-0.79886900
H	0.42116200	-3.02925900	0.94161800
Ni	-0.06358000	-0.02280500	-0.15347000
C	2.06556500	-0.25149600	0.94592600
C	2.92230800	0.40492800	0.07951600
H	2.81971800	1.48562600	-0.00759100
C	3.38427800	-0.32841100	-1.14230300
C	2.26727900	-0.61682100	-2.19223200
O	2.62450500	-0.81379800	-3.36185400
O	1.04644400	-0.67613600	-1.78766600
C	0.98257900	0.28182800	1.68303900
H	0.94639300	1.35824800	1.84679300
H	3.78232200	-1.31360800	-0.86320100
C	4.82187500	0.41238200	1.62233300
O	4.57631600	1.38335900	2.23992100
O	5.39472400	-0.54680600	1.25279100
H	4.18962200	0.18803100	-1.67046300
H	0.55690900	-0.31148200	2.48800900
H	2.15470200	-1.33990500	0.95704300

Int-Me

Thermal Correction to Free Energy: 0.288011 Hartree
SCF energy: -1129.359625 Hartree
Gibbs free energy: -1129.071614 Hartree
Coordinates:

C	1.64875700	-2.31027600	-0.69719900
C	2.18276100	-0.05948300	-0.18488200
C	3.50681900	-0.44013500	0.12876800
C	3.88364900	-1.75856500	0.02751100
C	2.93545300	-2.71665900	-0.40794500
H	4.22294600	0.30605400	0.44776100
H	4.89660000	-2.06103300	0.26650600
H	3.21298500	-3.75622900	-0.52966000
C	1.69353900	1.29259600	-0.16763100
C	2.47294600	2.42183500	0.16966100
C	1.91563900	3.67784100	0.11591600
H	3.50633200	2.29801000	0.46620500
C	-0.17244900	2.68673500	-0.57708600
C	0.56426000	3.81724400	-0.27476400
H	2.50598500	4.55187400	0.36608300
H	0.10186600	4.79433400	-0.33926100
N	1.25899100	-1.01232000	-0.57403700
N	0.36975900	1.44327700	-0.53283100
C	0.60573500	-3.26505000	-1.20799900
H	1.00513800	-4.27348000	-1.32127300
H	-0.25081100	-3.30235100	-0.53177900
H	0.23090500	-2.92113500	-2.17752100
C	-1.62498900	2.77229900	-0.95580400
H	-1.89147700	3.77893700	-1.28104400
H	-1.86006700	2.05323400	-1.74221500
H	-2.25299400	2.51277700	-0.09858200
Ni	-0.60347400	-0.32215800	-0.55097500
C	-0.77876100	0.28641300	2.19801400
C	-1.49896900	-0.61176000	1.31077100
C	-2.94099100	-0.20495500	1.00317500
C	-3.38349600	-0.51430200	-0.43766600
O	-4.56987000	-0.73348200	-0.69808300
O	-2.43652500	-0.47862500	-1.32522200
H	-3.05662500	0.87977600	1.11730600
C	0.18029000	-0.00386800	3.10651700
H	0.49947800	-1.02195900	3.30382900
H	-3.67093700	-0.66079000	1.68824900
H	0.69404600	0.78220100	3.64941100
H	-1.02347300	1.34114100	2.06297400
C	-1.39219000	-2.09368700	1.64974600

H	-0.35444400	-2.43866700	1.66459800
H	-1.82493300	-2.31839000	2.63981200
H	-1.93133100	-2.70105400	0.91579100

TS1-Me

Thermal Correction to Free Energy: 0.294052 Hartree

SCF energy: -1318.001864 Hartree

Gibbs free energy: -1317.707812 Hartree

Coordinates:

C	1.91004400	-2.15046600	-1.17352500
C	2.32937500	-0.14759800	0.00786100
C	3.46244000	-0.72736200	0.61201800
C	3.80041200	-2.02992100	0.32028700
C	3.01359200	-2.75328800	-0.60164200
H	4.06269100	-0.15226800	1.30432500
H	4.66636100	-2.49024300	0.78114500
H	3.27516400	-3.76709500	-0.87768000
C	1.91338700	1.22484200	0.19957600
C	2.58599600	2.15237600	1.01871700
C	2.12297600	3.44701400	1.10406000
H	3.46164100	1.85039600	1.57752500
C	0.33606300	2.87157200	-0.40975700
C	0.97807300	3.81683700	0.36955300
H	2.63315000	4.17307100	1.72610400
H	0.59630900	4.82942000	0.40924900
N	1.55141800	-0.87469000	-0.86366700
N	0.79353500	1.59635400	-0.50601400
C	1.06948700	-2.84682600	-2.20722400
H	1.46630600	-3.83392600	-2.44595200
H	0.03922800	-2.95899300	-1.86460800
H	1.03733900	-2.24640400	-3.12210200
C	-0.91599100	3.19384800	-1.17545600
H	-1.04106200	4.27046500	-1.29742900
H	-0.90466500	2.70743700	-2.15238700
H	-1.79096700	2.80559200	-0.64518600
Ni	-0.19117500	-0.00089800	-1.23470900
C	-1.04206600	-0.01540700	1.30128100
C	-1.65283700	-0.65958200	0.19990900
C	-2.90688500	-0.03517200	-0.39513600
C	-2.89888500	0.06455200	-1.93261500
O	-3.95739600	0.05288800	-2.56422700
O	-1.72661300	0.20426800	-2.47308900
H	-3.02432400	0.99272600	-0.03208100
C	-1.87430400	-0.89207100	3.80206800

O	-1.94172000	0.14266100	4.37490400
O	-2.18640000	-2.01485000	3.58828300
C	-0.19361900	-0.53702800	2.26505500
H	0.17973500	-1.55085700	2.18243700
H	-3.81765400	-0.57117800	-0.09723500
H	0.38931500	0.14088200	2.87645100
H	-1.26773900	1.04629800	1.39525500
C	-1.64997300	-2.17816300	0.14483400
H	-0.66310800	-2.59417400	0.36039600
H	-2.35168600	-2.59916800	0.87800700
H	-1.95518900	-2.53173200	-0.84460800

TS2-Me

Thermal Correction to Free Energy: 0.291628 Hartree

SCF energy: -1317.994770 Hartree

Gibbs free energy: -1317.703142 Hartree

Coordinates:

C	2.02039000	2.57060300	0.21798000
C	2.98490100	0.46304100	-0.26738800
C	4.18929100	1.09678800	-0.64522200
C	4.29594600	2.46658400	-0.57273500
C	3.18891400	3.22301600	-0.12294700
H	5.02703400	0.50669200	-0.99261400
H	5.21748500	2.96110400	-0.85679200
H	3.24757800	4.30112600	-0.04259800
C	2.77570300	-0.96222100	-0.28256200
C	3.77128400	-1.90456000	-0.62348800
C	3.48752000	-3.24947200	-0.56731500
H	4.75776000	-1.57033600	-0.91596800
C	1.23841400	-2.71336900	0.12285700
C	2.19778300	-3.66635000	-0.17632100
H	4.24770900	-3.98109200	-0.81572500
H	1.94830000	-4.71797100	-0.11182500
N	1.90687900	1.21796500	0.15290200
N	1.51109300	-1.38532200	0.07994300
C	0.79796000	3.31073700	0.68140300
H	0.42634600	2.88275500	1.61703600
H	1.00048800	4.37158000	0.83066500
H	-0.00512600	3.20703900	-0.05491500
C	-0.16594100	-3.11204300	0.48722000
H	-0.19384800	-4.12621100	0.88875900
H	-0.58979200	-2.41456300	1.21043400
H	-0.80364100	-3.08626200	-0.40186700
Ni	0.22002000	0.15906400	0.28804600

C	-1.92378400	-0.16304300	-0.93409400
C	-2.89325000	0.44828700	-0.16099700
C	-3.32901800	-0.30493800	1.06348500
C	-2.28758500	-0.19223600	2.21948800
O	-2.70943100	-0.15894100	3.38290100
O	-1.03834800	-0.16126400	1.90287500
C	-0.80206200	0.43853500	-1.56443200
H	-0.82109000	1.51110400	-1.74960300
H	-3.43238700	-1.37384000	0.84118800
C	-4.64007500	-0.11257300	-1.83766500
O	-4.65176500	0.89617400	-2.44135500
O	-4.92333500	-1.19845700	-1.48618800
H	-4.28648200	0.03879100	1.46512900
H	-0.27430300	-0.12834000	-2.32889400
H	-1.93013200	-1.25196500	-0.91873400
C	-2.93882600	1.95043400	-0.06021200
H	-2.87502100	2.42163800	-1.04426600
H	-3.86643600	2.28675700	0.41353200
H	-2.10315300	2.33628700	0.54364900

S-d2’

Thermal Correction to Free Energy: 0.461794 Hartree

SCF energy: -1631.536654 Hartree

Gibbs free energy: -1631.074860 Hartree

Coordinates:

C	-1.54802900	-3.10362700	-0.45519700
C	-1.45091000	-0.80098700	-0.36203000
C	-2.79924600	-0.69067200	0.04451200
C	-3.55064900	-1.89605700	0.17695900
C	-2.88986500	-3.09340900	-0.06084000
H	-3.41854300	-4.03394300	0.02728100
C	-0.63532000	0.37012300	-0.53550600
C	-1.16891000	1.64502400	-0.25496800
C	-0.31274100	2.76786300	-0.44990800
C	1.40717800	1.21994600	-1.22616300
C	0.95125000	2.52515500	-0.95699100
H	1.62603600	3.35413600	-1.12922200
N	-0.83924600	-1.98994600	-0.61825300
N	0.63427900	0.15537000	-0.98766100
C	2.78379500	0.98558300	-1.76475500
H	3.43740600	0.59835700	-0.97850900
H	2.75377100	0.22061700	-2.54183200
H	3.21659200	1.90404300	-2.16207100
Ni	1.04277200	-1.82124100	-1.12323900

C	3.75818200	-2.18530000	-0.44039800
H	3.44314100	-2.53792800	0.54092800
C	2.85710000	-2.51992200	-1.52193200
H	3.21353000	-2.28040400	-2.52529200
C	1.83386800	-3.53374400	-1.36446900
H	1.85687100	-4.16420300	-0.47106000
H	1.51256900	-4.08074500	-2.25291100
C	4.90766700	-1.47219800	-0.53895600
H	5.22139200	-1.15264700	-1.53130200
C	5.78659600	-1.06427900	0.55333900
C	6.99756400	-0.40514100	0.25597000
C	5.49369000	-1.28340300	1.91717400
C	7.87218600	0.00336000	1.25887100
H	7.24998300	-0.21589500	-0.78289500
C	6.36932500	-0.87767500	2.91736300
H	4.56685900	-1.77031600	2.19796700
C	7.56715300	-0.23126700	2.59964200
H	8.79536600	0.50707600	0.99209300
H	6.11391100	-1.06137700	3.95582500
H	8.24555300	0.08606400	3.38328100
H	-1.02947800	-4.03128600	-0.66018600
C	-0.72594200	4.15866300	-0.13683200
C	-1.19465600	4.50200900	1.13951600
C	-0.60684200	5.16243200	-1.10764600
C	-1.53806500	5.81857700	1.43489400
H	-1.27071500	3.73936300	1.90576900
C	-0.95951500	6.47702600	-0.81257300
H	-0.25027100	4.90629300	-2.09875700
C	-1.42550700	6.80875900	0.45907300
H	-1.88967600	6.07113500	2.42857400
H	-0.87150400	7.24104000	-1.57637500
H	-1.69746700	7.83241300	0.68912700
C	-4.98782400	-1.90952800	0.54630600
C	-5.43024500	-2.70049200	1.61551800
C	-5.93008100	-1.17556500	-0.18872700
C	-6.78134100	-2.74603100	1.94993700
H	-4.70970400	-3.26803200	2.19322900
C	-7.28142200	-1.22942200	0.14199900
H	-5.60437300	-0.57811700	-1.03216100
C	-7.71048200	-2.01109100	1.21447600
H	-7.10738700	-3.35441900	2.78564300
H	-7.99921600	-0.66411700	-0.44108700
H	-8.76222600	-2.04885900	1.47358300
C	-2.53418400	1.72988600	0.17503600

C	-3.31003900	0.62035000	0.32111000
H	-2.95572800	2.70407600	0.38140400
H	-4.33196300	0.72475600	0.65820900

T-TS3'

Thermal Correction to Free Energy: 0.466050 Hartree

SCF energy: -1820.160566 Hartree

Gibbs free energy: -1819.694517 Hartree

Coordinates:

C	0.14916000	-2.79891400	-0.33071300
C	-0.70050500	-0.65419200	-0.32413300
C	-2.03243000	-1.11250100	-0.46062100
C	-2.24192600	-2.51514400	-0.56493500
C	-1.12590800	-3.34273900	-0.48413200
H	-1.23671400	-4.41673500	-0.55833800
C	-0.41659700	0.75171700	-0.25303600
C	-1.47009600	1.69177300	-0.24161800
C	-1.11941600	3.06752200	-0.15222500
C	1.22351200	2.40042500	-0.16915900
C	0.23363800	3.39005300	-0.13939300
H	0.53604700	4.42748000	-0.07466800
N	0.37159500	-1.49065600	-0.26007300
N	0.89849400	1.10190700	-0.21241000
C	2.68478800	2.73384300	-0.12035700
H	3.10640900	2.41365600	0.83783700
H	3.22342500	2.18829000	-0.89972200
H	2.86131300	3.80232700	-0.23990400
Ni	2.10311700	-0.46136200	0.00901400
C	2.48690900	-2.11423400	2.27282400
H	2.15977100	-3.04251200	1.80940100
C	3.34709900	-1.29617800	1.50517700
H	3.77001700	-0.43205800	2.01499300
C	3.80695100	-1.62233500	0.19243400
H	3.56951800	-2.61608400	-0.18383400
C	0.03241100	-1.00698500	2.93930000
O	-0.69376000	-1.95193800	2.86379700
O	0.19338200	0.17151600	2.83121800
C	1.95378300	-1.79780600	3.51930700
H	1.52842400	-2.59031200	4.12302700
H	2.35460600	-0.94606700	4.06088300
C	4.87244000	-0.92724100	-0.52426400
C	5.31726700	-1.43316400	-1.76762600
C	5.48579500	0.25913600	-0.05696400
C	6.30327200	-0.78904700	-2.50351100

H	4.86830800	-2.34359500	-2.15239000
C	6.47013600	0.90156300	-0.79904200
H	5.18150100	0.68697100	0.89057900
C	6.88857600	0.38903800	-2.02925500
H	6.61951800	-1.20666500	-3.45369000
H	6.91709800	1.81157200	-0.41245900
H	7.65689900	0.89316400	-2.60377300
H	1.02044900	-3.43944300	-0.27061100
C	-2.12848700	4.15087800	-0.06318300
C	-2.07062600	5.24216400	-0.94145200
C	-3.12202600	4.13141400	0.92697200
C	-2.99260900	6.28103500	-0.84141000
H	-1.30907200	5.26558600	-1.71257600
C	-4.03785900	5.17492500	1.03018700
H	-3.16141400	3.30697300	1.62924000
C	-3.97885000	6.25051300	0.14415500
H	-2.94128400	7.11315100	-1.53417400
H	-4.79401500	5.15001700	1.80639500
H	-4.69458000	7.06059900	0.22330500
C	-3.58633400	-3.11403900	-0.75033900
C	-4.03157800	-4.11689700	0.12198900
C	-4.41302700	-2.72561700	-1.81459700
C	-5.27987000	-4.70757300	-0.05779300
H	-3.40215300	-4.41950400	0.95106900
C	-5.65706500	-3.32352500	-1.99727500
H	-4.07126600	-1.96788700	-2.51000500
C	-6.09584900	-4.31294800	-1.11759500
H	-5.61526200	-5.47441500	0.63093100
H	-6.28145900	-3.01923700	-2.82940100
H	-7.06627600	-4.77464900	-1.25857000
C	-2.81315700	1.19713000	-0.34716800
C	-3.08094600	-0.13325400	-0.45232200
H	-3.63087700	1.90466800	-0.35301200
H	-4.10724500	-0.46530600	-0.52501000

T-TS4’

Thermal Correction to Free Energy: 0.469769 Hartree

SCF energy: -1820.161610 Hartree

Gibbs free energy: -1819.691841 Hartree

Coordinates:

C	-2.20963100	-0.40758900	-2.20625800
C	-0.19097100	0.31507800	-1.35280600
C	-0.71299400	1.58574400	-1.01649600
C	-2.08371600	1.83626700	-1.31364000

C	-2.81475200	0.81469500	-1.90868200
H	-3.85735700	0.96290400	-2.15763300
C	1.17676700	-0.01650800	-1.05483900
C	2.00315300	0.91826500	-0.39829300
C	3.32915800	0.50982400	-0.08390500
C	2.84015300	-1.63718200	-1.12069800
C	3.72339000	-0.76219900	-0.47032500
H	4.72082100	-1.10957900	-0.23335000
N	-0.93586600	-0.66224500	-1.93055800
N	1.59076700	-1.26200800	-1.40896100
C	3.23081800	-3.04302000	-1.46224300
H	2.71035500	-3.72182500	-0.78070000
H	2.91835900	-3.28834000	-2.48065900
H	4.30509100	-3.19921900	-1.36752000
Ni	0.09493300	-2.42861200	-2.09092100
C	-1.63103800	-3.17514800	-0.10711400
H	-2.36232500	-2.48582900	-0.51707700
C	-0.94679300	-3.97413500	-1.03550200
H	-0.20051200	-4.65880600	-0.63461100
C	-1.16385900	-3.97468800	-2.45307900
H	-2.11093700	-3.60202500	-2.83994800
H	-0.74791100	-4.80199300	-3.02113100
C	0.48952300	-2.24913100	1.43855200
O	0.34790000	-1.07784600	1.64292300
O	1.26471000	-3.14864500	1.25763900
C	-1.43143700	-3.14287000	1.29881400
H	-1.07210200	-4.05876200	1.76099400
C	-2.28873900	-2.30482100	2.14534300
C	-2.64504500	-2.71327100	3.44379700
C	-2.73227000	-1.03631800	1.71881900
C	-3.42559600	-1.90710100	4.26816400
H	-2.30693000	-3.68038300	3.80340900
C	-3.51360500	-0.23219500	2.54195300
H	-2.43316400	-0.66496200	0.74600500
C	-3.87013700	-0.66071500	3.82244200
H	-3.68967000	-2.25324500	5.26206800
H	-3.83136900	0.74367900	2.18935600
H	-4.47584200	-0.03110400	4.46439900
C	1.45210100	2.20280200	-0.07938000
C	0.15880400	2.51837000	-0.36282900
H	2.08277100	2.93462400	0.40630300
H	-0.22625100	3.48897200	-0.08365600
H	-2.77199300	-1.20924400	-2.66933300
C	4.27642900	1.37273400	0.66443700

C	3.93957200	1.87553800	1.92928900
C	5.54357400	1.65281000	0.13639500
C	4.84944200	2.64860900	2.64547100
H	2.97200400	1.63988700	2.35696700
C	6.44863100	2.43381300	0.85105800
H	5.81090300	1.26784600	-0.84108800
C	6.10393000	2.93377700	2.10641100
H	4.57999200	3.02384400	3.62592300
H	7.42195700	2.65210800	0.42696200
H	6.80988400	3.53934600	2.66291600
C	-2.75305300	3.12245100	-0.99881400
C	-3.92965200	3.12270600	-0.23677300
C	-2.25689400	4.34123800	-1.48203700
C	-4.58662000	4.31677600	0.04889400
H	-4.32036000	2.18496900	0.14165900
C	-2.92074300	5.53294800	-1.20279200
H	-1.36183000	4.35192800	-2.09286300
C	-4.08398300	5.52478700	-0.43334200
H	-5.48912500	4.30287300	0.64890900
H	-2.53126200	6.46722300	-1.59029300
H	-4.59656900	6.45398100	-0.21308000

D-In6’

Thermal Correction to Free Energy: 0.470999 Hartree

SCF energy: -1820.326638 Hartree

Gibbs free energy: -1819.855639 Hartree

Coordinates:

C	-0.65296700	3.01176700	0.57106700
C	0.62181400	1.20272000	1.28833100
C	1.79124000	2.00900200	1.39605000
C	1.70371800	3.37177000	1.04111500
C	0.43641500	3.85742400	0.64092900
H	0.32065300	4.89430200	0.35127900
C	0.66260900	-0.18503600	1.56759200
C	1.86377100	-0.80669500	2.00387200
C	1.85047300	-2.20211800	2.20548500
C	-0.48792500	-2.22080100	1.50498300
C	0.65279800	-2.88939800	1.93504300
H	0.60782900	-3.96139000	2.08243900
N	-0.59908200	1.70442800	0.88708700
N	-0.50336000	-0.88402200	1.34150100
C	-1.75191300	-2.96063400	1.17126200
H	-1.76541300	-3.95378800	1.62194300
H	-2.62579500	-2.39164200	1.49188500

H	-1.83793000	-3.07476800	0.08575300
Ni	-1.84987100	0.26410500	0.36207400
C	-0.18273600	-0.44059100	-1.69971200
H	-0.04554400	-1.50699100	-1.51931100
C	-1.54340100	-0.00563400	-1.69905300
H	-1.70454500	1.00833300	-2.07923900
C	-2.65257200	-0.98012600	-2.06256700
H	-2.27388600	-2.00851900	-1.99897300
H	-3.01926800	-0.86050400	-3.08941100
C	-3.87742400	-0.94149400	-1.12615500
O	-4.96521000	-1.37461900	-1.51336000
O	-3.66143300	-0.47714000	0.06713400
C	0.93901400	0.34087200	-1.78035300
H	0.79615800	1.40363900	-1.96924900
C	2.31078600	-0.07275500	-1.56955800
C	3.35836400	0.85468300	-1.78434000
C	2.69170400	-1.36240700	-1.12663300
C	4.69080500	0.52137000	-1.57165000
H	3.10525400	1.85803200	-2.11374300
C	4.02397100	-1.69330500	-0.91857300
H	1.92984600	-2.09948300	-0.90219200
C	5.04105900	-0.75848300	-1.13523300
H	5.46160500	1.26712500	-1.74149400
H	4.27214800	-2.68583600	-0.55690500
H	6.07860400	-1.01990700	-0.96006200
H	-1.61772600	3.37592700	0.23443300
C	2.98550400	1.36063700	1.86586100
C	3.02125800	0.03180300	2.14629500
H	3.88489300	1.94876200	1.98584700
H	3.95408900	-0.41619000	2.45957800
C	3.03723200	-2.97018800	2.64953300
C	3.75501900	-2.62438100	3.80515900
C	3.44864600	-4.10097600	1.92583900
C	4.85449500	-3.37555400	4.21442300
H	3.43610000	-1.77247600	4.39431100
C	4.54927600	-4.85020900	2.33303400
H	2.90850000	-4.38035500	1.02842000
C	5.25894200	-4.48947300	3.47873500
H	5.39112400	-3.09412300	5.11366000
H	4.85586100	-5.71338900	1.75273400
H	6.11581800	-5.07222600	3.79693400
C	2.86173600	4.29515000	1.04243800
C	2.75968400	5.55691100	1.65192900
C	4.06525400	3.96796100	0.39385100

C	3.82636400	6.45175900	1.62970900
H	1.84022600	5.82805400	2.15888400
C	5.13094000	4.86388200	0.37171300
H	4.15188500	3.01379200	-0.11155900
C	5.01863900	6.10894200	0.99136000
H	3.72773300	7.41660100	2.11489700
H	6.04769600	4.59206100	-0.14000100
H	5.84868000	6.80600000	0.97297100

D-TS6'

Thermal Correction to Free Energy: 0.478942 Hartree

SCF energy: -2008.967542 Hartree

Gibbs free energy: -2008.488600 Hartree

Coordinates:

C	-0.42553700	-2.95065100	-1.52244700
C	0.25762500	-0.74886200	-1.26848200
C	1.61010400	-1.13277100	-1.07194400
C	1.92056400	-2.51381100	-1.08737100
C	0.86940100	-3.41073100	-1.33628400
H	1.05766200	-4.47677700	-1.34952000
C	-0.13274400	0.61668000	-1.19885800
C	0.82775800	1.63243800	-0.97064000
C	0.36375000	2.96422900	-0.86217800
C	-1.90873500	2.13071700	-1.16857800
C	-1.01716700	3.17951000	-0.95630400
H	-1.40613500	4.18728400	-0.87882700
N	-0.75091100	-1.65135600	-1.49367700
N	-1.47727200	0.86349700	-1.31075400
C	-3.39250600	2.35281900	-1.22024900
H	-3.63564600	3.39858500	-1.41074700
H	-3.84827100	1.71702600	-1.98123200
H	-3.84160300	2.06587200	-0.26317900
Ni	-2.54920500	-0.84371700	-1.33057200
C	-2.37321600	-0.65649400	1.27398700
H	-2.62406500	0.39109700	1.43122800
C	-3.33559800	-1.41304600	0.61262800
H	-3.17556600	-2.49195800	0.57169600
C	-4.77383700	-0.95890200	0.48357500
C	-5.32452300	-0.93804700	-0.95763700
O	-6.53805800	-1.01094900	-1.15442100
O	-4.43839500	-0.79428100	-1.89620900
H	-4.86943300	0.07151600	0.84837200
C	-2.02634500	-1.62055100	3.74900700
O	-1.90601100	-0.65712200	4.43879800

O	-2.38965900	-2.74645900	3.59901000
C	-1.13631400	-1.10571900	1.78565300
H	-0.86558000	-2.12845900	1.53720000
H	-5.45631000	-1.56219200	1.09188200
C	-0.00968500	-0.24182600	2.12488100
C	1.24647300	-0.82319200	2.40708000
C	-0.10104500	1.15998200	2.24877100
C	2.33660100	-0.05687400	2.79914000
H	1.35644200	-1.89905700	2.30961300
C	0.99318900	1.92640700	2.63517300
H	-1.03245800	1.66252400	2.01750000
C	2.22267300	1.33029000	2.91861500
H	3.28521200	-0.54223500	3.00720100
H	0.88906500	3.00425800	2.70045300
H	3.07423100	1.93272700	3.21411700
H	-1.24482500	-3.64234200	-1.68227800
C	2.56601600	-0.08237100	-0.86502900
C	2.19438100	1.22398800	-0.80937700
H	3.60736200	-0.34193700	-0.73421600
H	2.94429200	1.97725800	-0.61218800
C	1.26247100	4.11875800	-0.62435300
C	2.37375000	4.36984100	-1.44361800
C	0.98928200	5.01305100	0.42227800
C	3.19250500	5.47300000	-1.21459000
H	2.58436000	3.70635600	-2.27420900
C	1.81031100	6.11361000	0.65345800
H	0.13612400	4.83087300	1.06535700
C	2.91692000	6.34692400	-0.16296200
H	4.04283600	5.65327500	-1.86261600
H	1.58793100	6.78658900	1.47393200
H	3.55650600	7.20355100	0.01622000
C	3.28089300	-3.04663200	-0.83448900
C	3.84606200	-3.98053000	-1.71649700
C	4.00997200	-2.67895000	0.30750200
C	5.10719200	-4.51856500	-1.47300900
H	3.29672500	-4.27296500	-2.60440200
C	5.26932900	-3.22050300	0.55184600
H	3.57532800	-1.98119800	1.01237100
C	5.82465000	-4.13978000	-0.33836600
H	5.53070600	-5.23164200	-2.17137300
H	5.81371300	-2.92940100	1.44319700
H	6.80568900	-4.55967900	-0.14794500

D-TS8’

Thermal Correction to Free Energy: 0.475727 Hartree
SCF energy: -2008.956768 Hartree
Gibbs free energy: -2008.481041 Hartree
Coordinates:

C	1.03547400	2.65712900	-1.20270000
C	-0.43307100	0.88478300	-0.95824900
C	-1.52583400	1.75285400	-0.70512000
C	-1.28022100	3.15219400	-0.70006800
C	0.01928500	3.57953600	-0.98313900
H	0.25361700	4.63673700	-0.99231800
C	-0.61155500	-0.53818200	-0.94380700
C	-1.88575100	-1.08919300	-0.67528300
C	-1.99021600	-2.50340300	-0.61208000
C	0.39993800	-2.62481700	-1.06413300
C	-0.83123200	-3.24168000	-0.79840200
H	-0.87158000	-4.32288900	-0.75144800
N	0.83795000	1.33383400	-1.17691700
N	0.50659000	-1.29519900	-1.16085600
C	1.64499900	-3.44979600	-1.21490800
H	1.41446600	-4.44425800	-1.60098300
H	2.36905600	-2.94750800	-1.85472100
H	2.11603400	-3.57346100	-0.23314000
Ni	2.20539500	-0.15197200	-1.09036300
C	3.16453300	-0.16982600	0.87942500
H	3.37312400	-1.22965000	1.03560400
C	4.18387900	0.56638700	0.23198300
H	4.01235700	1.61914600	0.02574300
C	5.29196300	-0.13616000	-0.50049900
C	4.92121000	-1.04712300	-1.70233300
O	5.84871600	-1.63453400	-2.27759500
O	3.68216100	-1.15206400	-2.03026100
C	1.98804200	0.35764000	1.43011200
H	1.85034000	1.42927800	1.32973000
H	5.86072600	-0.77806700	0.18373300
C	5.27342800	1.25309900	2.27494800
O	4.56118300	2.12765900	2.62089500
O	6.19128900	0.51223400	2.31673500
H	6.02088100	0.58608700	-0.88099500
C	0.88081800	-0.35575100	1.99321900
C	-0.31283400	0.35031500	2.30265800
C	0.84477500	-1.76380800	2.18265800
C	-1.45680500	-0.29985900	2.74423800
H	-0.33216200	1.42567900	2.15653200
C	-0.30316800	-2.40520300	2.62087100

H	1.72362100	-2.35544000	1.95286000
C	-1.47261400	-1.68757100	2.90166200
H	-2.35301000	0.27847900	2.94448200
H	-0.29667900	-3.48548100	2.72979900
H	-2.37110600	-2.20073900	3.22345400
C	-2.80934900	1.15930200	-0.46609500
C	-2.97578600	-0.19053300	-0.43960700
H	-3.65994300	1.80389600	-0.29210400
H	-3.95250200	-0.60085000	-0.22239900
C	-3.26754600	-3.20779300	-0.33675200
C	-4.40154400	-3.00806200	-1.13652900
C	-3.34140400	-4.12445900	0.72146200
C	-5.58136100	-3.70265700	-0.87899600
H	-4.35205700	-2.31807400	-1.97091500
C	-4.52253900	-4.81538900	0.98047500
H	-2.47219200	-4.27467000	1.35062600
C	-5.64667400	-4.60584500	0.18166400
H	-6.44767100	-3.54170400	-1.51053200
H	-4.56612900	-5.51367800	1.80864400
H	-6.56613500	-5.14346700	0.38311800
C	-2.32490100	4.15668000	-0.38386600
C	-2.55843200	5.22976500	-1.25615600
C	-3.05884700	4.08975000	0.81044000
C	-3.50844100	6.20122700	-0.95019800
H	-1.99977300	5.29186700	-2.18328400
C	-4.00491500	5.06429200	1.11755600
H	-2.87041200	3.28140600	1.50744600
C	-4.23564000	6.12148000	0.23714800
H	-3.68213500	7.01901900	-1.64041900
H	-4.55724900	5.00121100	2.04829700
H	-4.97388900	6.87831700	0.47617400
H	2.05480000	2.98128700	-1.37618300

S-TS3' (**S-TS3** with the full ligand)
Thermal Correction to Free Energy: 0.470208 Hartree
SCF energy: -1820.156545 Hartree
Gibbs free energy: -1819.686337 Hartree
Coordinates:

C	-0.68466500	-3.01829700	-0.60222500
C	0.23081100	-0.89624300	-0.69660200
C	1.55013100	-1.40981400	-0.62485600
C	1.71849100	-2.81998900	-0.52442200
C	0.57908900	-3.61019100	-0.56306600
H	0.65616200	-4.68795600	-0.49799700

C	0.01483200	0.53201100	-0.78732600
C	1.11991100	1.41352500	-0.74415400
C	0.83943000	2.81176900	-0.74437600
C	-1.52056700	2.25604700	-0.87222300
C	-0.48420300	3.20732100	-0.78598900
H	-0.73234600	4.26210000	-0.78069400
N	-0.86951100	-1.69958800	-0.63158900
N	-1.26738500	0.95505700	-0.88400600
C	-2.96004700	2.68415000	-0.94167300
H	-3.59112300	1.82299000	-1.15715500
H	-3.27196800	3.11456500	0.01575400
H	-3.10837500	3.45151600	-1.70576800
Ni	-2.56175800	-0.86127900	-0.07967000
C	-3.67542400	-0.22916500	1.44398100
H	-3.79063300	0.85166100	1.41597800
C	-4.83221700	-1.01631800	1.18563600
H	-4.76383100	-2.07373100	1.43922400
C	-5.96693900	-0.59249500	0.52730400
H	-6.13607200	0.46814000	0.36162300
H	-6.83083800	-1.24001100	0.45761400
C	-5.27605500	-0.95217100	-1.64199300
O	-6.27176500	-1.26869100	-2.18795900
O	-4.10518700	-0.70864600	-1.61982400
C	-2.43525300	-0.83245900	1.85741400
H	-2.48209000	-1.85627500	2.23453000
C	-1.24820400	-0.08096500	2.30858500
C	-1.20376600	1.32178400	2.39397900
C	-0.05899700	-0.78441100	2.57942200
C	-0.02197900	1.98702800	2.70709100
H	-2.09623600	1.90129100	2.19290300
C	1.12290900	-0.12000500	2.88712600
H	-0.06315400	-1.86738200	2.50636600
C	1.15193900	1.27408100	2.94865100
H	-0.01565800	3.07056500	2.75199400
H	2.02731000	-0.69081000	3.06893100
H	2.07499100	1.79603400	3.17326200
H	-1.58099300	-3.62420700	-0.56084600
C	1.90957400	3.84024200	-0.67209600
C	2.92167800	3.91153500	-1.63912800
C	1.89551400	4.78358300	0.36379700
C	3.89829100	4.90197000	-1.56798700
H	2.93303900	3.19804600	-2.45498400
C	2.87678600	5.76957600	0.43754200
H	1.11889400	4.73250600	1.11809800

C	3.88085300	5.83134400	-0.52789600
H	4.67054600	4.94958700	-2.32718300
H	2.85767900	6.48716800	1.24980300
H	4.64390000	6.59911700	-0.47177300
C	3.04637000	-3.45991800	-0.34773400
C	3.46733000	-4.46981000	-1.22273000
C	3.87324200	-3.10650800	0.72843900
C	4.69436100	-5.10196200	-1.03445100
H	2.83549500	-4.74898300	-2.05825900
C	5.09521400	-3.74544100	0.91980600
H	3.54740800	-2.34188100	1.42412500
C	5.51122100	-4.74184500	0.03670500
H	5.01176700	-5.87494000	-1.72488800
H	5.72001700	-3.46794400	1.76094900
H	6.46453000	-5.23606300	0.18418000
C	2.43781400	0.86036000	-0.66645900
C	2.64333600	-0.48338900	-0.63295900
H	3.28672800	1.52914300	-0.62965300
H	3.65309800	-0.86760500	-0.59474600