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Theoretical Investigation of Mechanism on Nickel-Catalyzed Electrochemical Cross-Coupling of Aryl Bromides and Arylamines

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Contents

Background.

Electrochemical systems have emerged as effective alternatives to conventional redox agents in nickel-catalyzed reductive cross-coupling reactions. Recently, we developed a reductive neutral cross-coupling reaction of aryl bromides and arylamines over nickel/bipyridine catalysts under mild conditions and a broad substrate scope. Terminal oxidants and sacrificial reducing agents can be avoided. Meanwhile, the role of electrolysis in the formation of carbon radicals and the regeneration of low-valent nickel complexes has been demonstrated through a divided-cell experiment and a radical trapping test, but the exact mechanism is still unclear. At the same time, the bipyridine ligands with different substituents showed completely different activities in the experiments, but we did not know the relationship between the ligands and the catalyst activity. Therefore, here we report the detailed mechanism of our nickel-catalyzed electrochemical aminomethylation of aryl bromides using density functional theory (DFT). The effects of catalyst ligands and their substituents on catalytic activity were also analyzed from steric effect analysis, ADCH (dipole moment corrected Hirshfeld population) charge analysis, and frontier molecular orbital (FMO) theory.

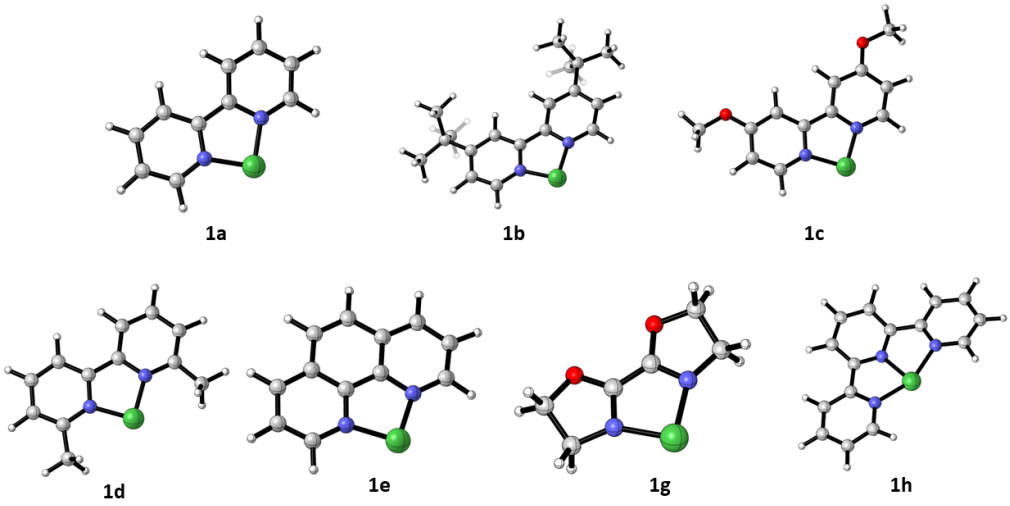

Fig. S1 Molecular structure of **1a-1e**, **1g-1h**.

Two pathways from **3f-s** and **3f-t** to the **CP-2f-s** product were compared. Starting with **3f-s**, the radical addition product is **5f'-s**. However, **5f'-s** can dissociate to form **3f-s** more easily (ΔG=4.8 kcal/mol) than undergoing reductive elimination to **CP-2f-s** with the energy barrier of 18.7 kcal/mol, suggesting the reversible radical addition process. Alternatively, via an intersystem crossing (ΔG=15.3 kcal/mol), **3f-t** is obtained from **3f-s** and undergoes radical addition to **5f-s** with a lower energy of 1.6 kcal/mol than that of **5f'-s**. And the corresponding reductive elimination energy barrier is only 7.1 kcal/mol. Therefore, the latter pathway is favorable.

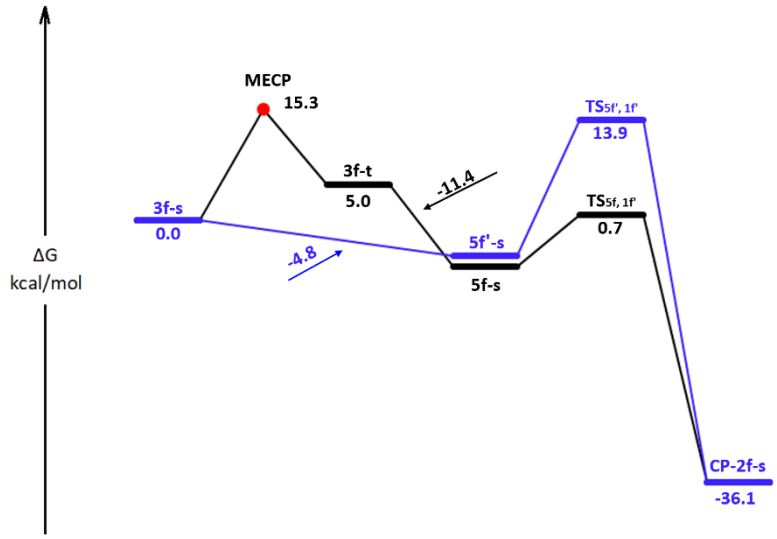

Fig. S2 Free energy profile for radical addition to **3f-s** and **3f-t**. Energies are in kcal/mol.

The presence of the radicals in the Ni(0) and Ni(I) catalysts was calculated (**Fig. S3**). Based on a relaxed potential energy surface scan on the Ni-C bond (**1f-t** to **III-f-s**; **1f'-s** to **III'-f-s; 3f-t** to **5f-s**), the barrierless process is presented. Though the oxidative addition of 4-bromotoluene only requires the energy barrier of 9.5 kcal/mol, its product **5f'-s** is difficult to continue the subsequent reductive elimination. Therefore, **5f'-s** dissociates the stable radicals to form **3f-s**. Comparing the free energy barrier of the rate-determining step, the radical addition on Ni(II) is more favorable than on Ni(0) or Ni(I).

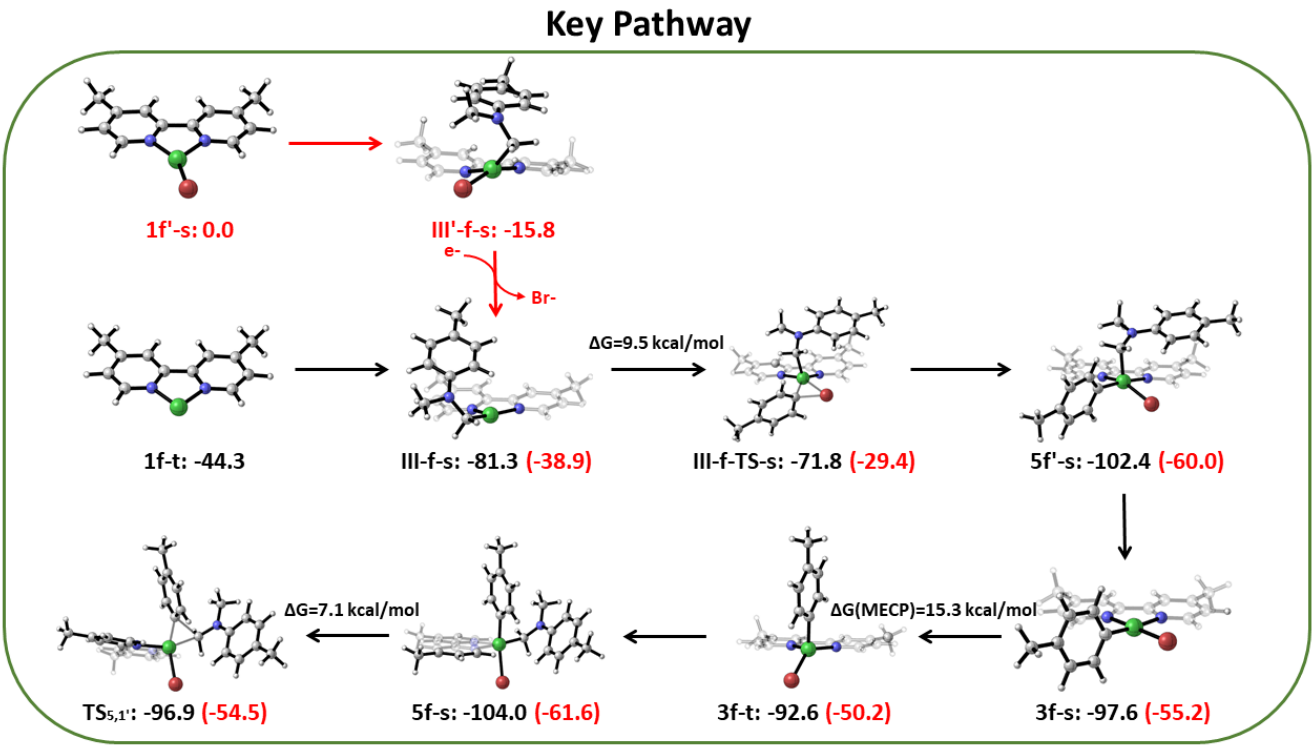

Fig. S3 Free energy profile for radical addition to the Ni(0)(black) and Ni(I)(red) catalyst (kcal/mol).

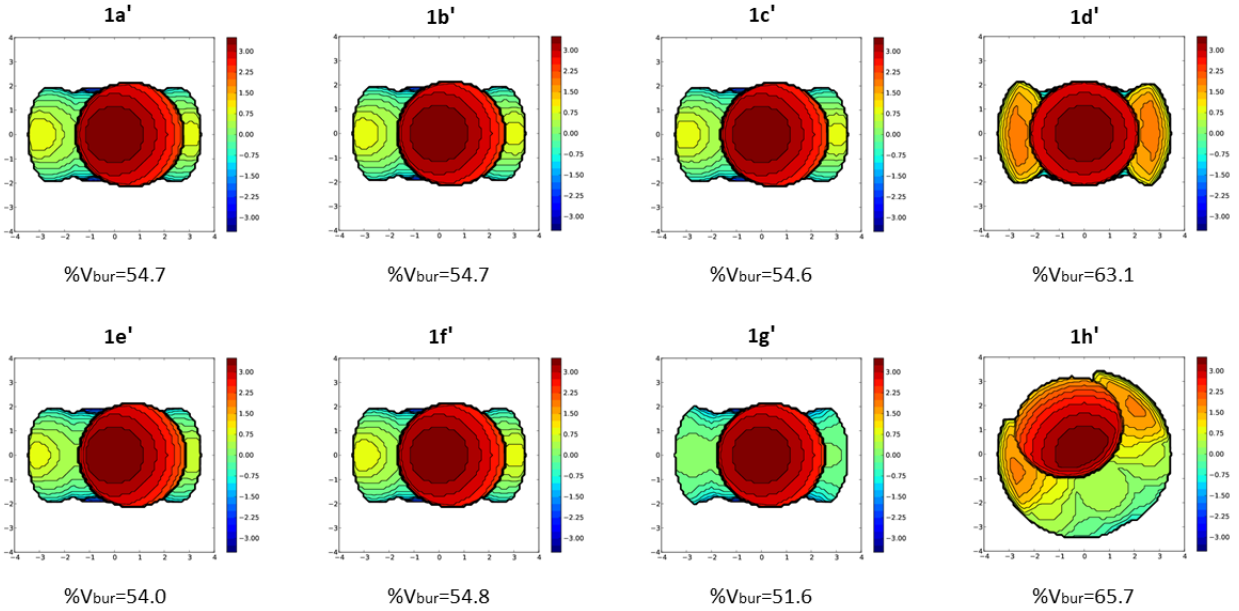

Fig. S4 Steric maps of the nickel catalysts **1a'-1h'**. The catalysts were oriented by placing the Ni atom at the origin of the sphere, with the mid-point between the N and N atom connecting the Ni atom aligned along the z-axis at negative z values and with two C atoms and one N atom in the xz-plane.

It should be noted that with Ni(0) as the starting point, by definition, the rate-determining step of the reaction should be the step of reductive elimination. However, through the calculation of the reaction mechanism of different catalysts, it is found that the reaction energy barriers of the two steps of oxidative addition and reductive elimination are similar, and oxidative addition is more subject to the ligands. Therefore, the oxidative addition steps of the two catalytic cycles are compared.

Table S1 Energy barriers (kcal/mol) of reductive elimination.

Entry	Ni Cat.	**5→TS$_{5,1'}$**
1	**a**	6.2
2	**b**	7.5
3	**c**	7.1
4	**d**	6.3
5	**e**	7.4
6	**f**	7.1

Calculation of reduction potential.

Equation (1) was concluded according to the previous studies[1-3].

$$E^{cal}_{1/2}(V\ vs\ SCE) = E_{Ox/Red} + E^{corr}_{1/2} + C_{DFT}$$

$$= -\frac{G[reduced]-G[oxidized]}{n_e F} + E^{SHE}_{1/2} + E^{SCE}_{1/2} + E_j + C_{DFT} \quad (1)$$

The "G" is the sum of the thermal correction to Gibbs free energy (298.15 K, 1 atm), the free energy of solvation, refined single point energy, and the free energy for the change of 1 atm/1M standard state (1.89 kcal/mol). Notably, the experimental solvation free energy[4] of Br^- in DMA was used in the calculation. The free energy of the electron (298.15 K, 1 atm) was considered from the reference[5]. The calculated redox potential is converted to SHE ($E^{SHE}_{1/2}$=-4.281 V) and then to SCE ($E^{SCE}_{1/2}$=-0.241 V *vs* SHE).[6] Since the correction factor E_j of DMA solvent in the calculations was not found, the value of DMF solvent[7] with similar properties was used in calculating the reduction potential.

According to the previous study[3], a training set to determine C_{DFT}(M06) was chosen based on the literature redox potentials (in V *vs* $Fc^{+/0}$ in CH_3CN). The Calculations were performed at the M06/def2-SVP//M06/def2-TZVPP (SMD, solvent=CH_3CN) level with disp3 dispersion corrections for a series of compounds. The total correction factor $E^{corr}_{1/2}$ is: -4.281 ($E^{SHE}_{1/2}$)-0.141 ($E^{SCE}_{1/2}$ *vs* SHE in CH_3CN)-0.400 ($E^{Fc}_{1/2}$ *vs* SCE in CH_3CN) = -4.822 V. **Fig. S5** shows the C_{DFT}(M06) by comparing the experimental and calculated values. The calculated redox potential with C_{DFT}(M06) shows no average deviation at +0.312 (**Table S2**).

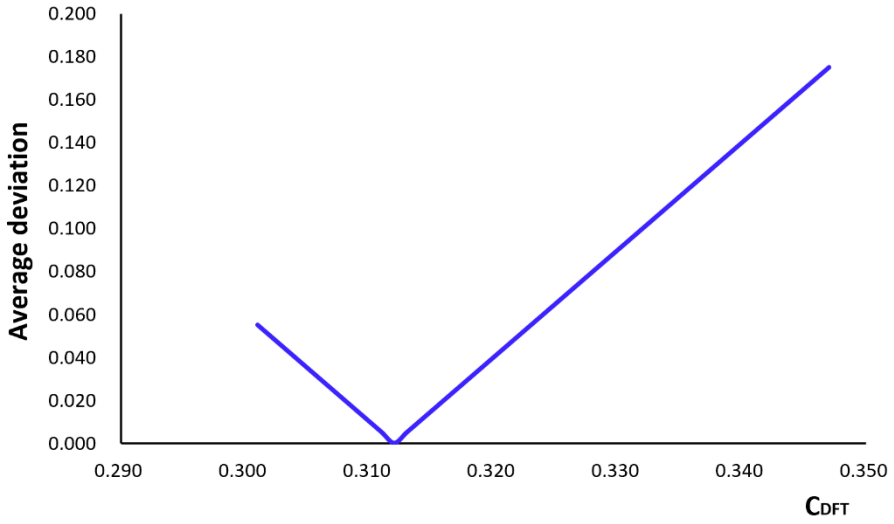

Fig. S5 Plot of average deviation vs C_{DFT}.

Table S2 Gibbs free energy, calculated redox potentials, and literature reported redox potentials. Calculations were performed at the M06/def2-SVP//M06/def2-TZVPP (SMD, CH_3CN) level with disp3 dispersion corrections(in V *vs* $Fc^{+/0}$ in CH_3CN) .

Compound	G_{298K} (kcal/mol)	Literature redox potential[3]	Calculated redox potential	Deviation
anethole	-463.1736	0.84	0.708	-0.132
[anethole]$^{\cdot+}$	-463.1736			
N(2,4,6-tribromophenyl)$_3$	-23910.4794	1.36	1.583	0.223
[N(2,4,6-tribromophenyl)$_3$]$^{\cdot+}$	-23910.4794			
N(4-bromophenyl)$_3$	-8469.8136	0.67	0.693	0.023
[N(4-bromophenyl)$_3$]$^{\cdot+}$	-8469.6202			
NEt_3	-292.2985	0.47	0.422	-0.048
[NEt_3]$^{\cdot+}$	-292.1287			
thianthrene	-1258.2883	0.86	0.794	-0.066
[thianthrenium]$^{\cdot+}$	-1258.1634			
average deviation				0.000

Taking **1f'**+e^-→**1f**+Br^- as an example.

$G_{1f'}$=-4656.1130 Hartree G_{e^-}=-3.616 kJ/mol

G_{1f}=-2081.9355 Hartree G_{Br^-}=-2574.2567 Hartree

$$E_{1/2}^{cal}(V\ vs\ SCE) = E_{Ox/Red} + E_{1/2}^{corr} + C_{DFT}$$

$$= -\frac{G[reduced]-G[oxidized]}{n_eF} + E_{1/2}^{SHE} + E_{1/2}^{SCE} + E_j(DMF) + C_{DFT}(M06)$$

=-(2625.5*(-2081.9385-2574.2567+4656.1160)+3.616[5])/96.5-4.281[6]-0.241[6]+0.172[7]+0.312

=-1.9207 V

ΔG(**1f'**→**1f**)=23.061*(-1.9207 V)=-44.3 kcal/mol

Energetics and the trend of HOMO of Ni(I) coordination complexes ahead of $TS_{1',3'}$.

The free energy and HOMOs of Ni(I) coordination complexes ahead of $TS_{1',3'}$ were calculated (**Table S3**). Only **CP-1h'** formed by 4-bromotoluene and **1h'** has a lower energy of 10.7 kcal/mol than reactants which results in a high energy barrier of 26.2 kcal/mol. Also, compared with the Ni(I) catalyst, all HOMO energy of **CP-1'** increases, but the correlation with the catalytic performance is not as obvious as uncoordinated Ni(I).

Table S3 Free energy profile and HOMO energy.

Entry	Ni Cat.	ΔG(**1'**→**CP-1'**)	HOMO energy
1	**1a'**	5.3	-5.398
2	**1b'**	10.8	-5.348
3	**1c'**	10.6	-5.327
4	**1d'**	7.1	-5.672
5	**1e'**	9.7	-5.500
6	**1f'**	4.0	-5.297
7	**1g'**	12.3	-5.483
8	**1h'**	-10.7	-5.100

Thermal correction to Gibbs Free Energy at M06-D3/def2-SVP, Energy at the M06-D3/def2-TZVPP level (Hartree), and Cartesian coordinates list.

1a-t

Geometry with 21 atoms:

Thermal correction to Gibbs Free Energy: 0.118268

Total energy: -2003.478013610

Ni	0.000004	1.898421	-0.000009
C	0.714708	-0.723777	-0.000021
C	1.523271	-1.892841	0.000054
C	2.893839	-1.790147	-0.000039
C	3.498340	-0.506759	-0.000203
C	2.665076	0.596910	-0.000230
C	-0.714711	-0.723776	0.000038
C	-1.523276	-1.892839	-0.000004
C	-2.893843	-1.790143	0.000076
C	-3.498343	-0.506753	0.000193
C	-2.665077	0.596914	0.000196
H	1.048663	-2.878314	0.000222
H	4.583686	-0.380719	-0.000287
H	3.086527	1.610316	-0.000331
H	-1.048669	-2.878313	-0.000137
H	-4.583689	-0.380713	0.000263
H	-3.086526	1.610321	0.000264
N	1.326760	0.523460	-0.000140
N	-1.326761	0.523461	0.000119
H	3.511453	-2.693780	0.000031
H	-3.511459	-2.693774	0.000031

1b-t

Geometry with 45 atoms:

Thermal correction to Gibbs Free Energy: 0.324424

Total energy: -2317.856379930

Ni	0.000028	3.204419	0.000126
C	-0.714788	0.580467	-0.000186
C	-1.523264	-0.587074	-0.000339
C	-2.903641	-0.520676	-0.000476
C	-3.490066	0.776991	-0.000346
C	-2.660746	1.885786	-0.000129
C	0.714839	0.580467	-0.000191
C	1.523308	-0.587078	-0.000290
C	2.903680	-0.520689	-0.000450
C	3.490118	0.776976	-0.000397
C	2.660806	1.885775	-0.000213
H	-1.029627	-1.564037	-0.000266
H	-4.571224	0.926387	-0.000429
H	-3.096016	2.893578	-0.000009
H	1.029669	-1.564044	-0.000141
H	4.571274	0.926369	-0.000509
H	3.096082	2.893564	-0.000146
N	-1.325984	1.828310	-0.000053
N	1.326042	1.828309	-0.000118
C	-3.736879	-1.801650	-0.000025
C	3.736849	-1.801699	0.000006
C	3.406273	-2.625489	-1.247312
H	4.009677	-3.550208	-1.270119
H	2.344558	-2.921095	-1.278296
H	3.625279	-2.057133	-2.168147
C	3.409814	-2.621540	1.250890
H	4.013159	-3.546278	1.274979
H	3.631470	-2.050238	2.169266
H	2.348089	-2.916731	1.285723
C	5.233981	-1.509549	-0.002653
H	5.543317	-0.941472	-0.896473
H	5.546272	-0.940053	0.889219
H	5.799166	-2.456984	-0.002769
C	-3.406107	-2.625711	-1.247110
H	-2.344414	-2.921413	-1.277820
H	-4.009579	-3.550389	-1.269855
H	-3.624880	-2.057521	-2.168103
C	-3.410270	-2.621310	1.251090
H	-3.632000	-2.049778	2.169303
H	-4.013809	-3.545923	1.275240
H	-2.348611	-2.916702	1.286198
C	-5.233969	-1.509356	-0.003110
H	-5.546379	-0.939478	0.888475
H	-5.543053	-0.941595	-0.897217
H	-5.799251	-2.456736	-0.002970

1c-t

Geometry with 29 atoms:

Thermal correction to Gibbs Free Energy: 0.175287

Total energy: -2232.496336920

Ni	-0.000000	2.569824	0.000111
C	-0.712774	-0.056476	-0.000243
C	-1.515554	-1.230684	-0.000293
C	-2.895320	-1.135475	-0.000204
C	-3.504524	0.146386	-0.000323
C	-2.659521	1.249863	-0.000222
C	0.712774	-0.056477	-0.000129
C	1.515553	-1.230686	-0.000129
C	2.895319	-1.135477	-0.000004
C	3.504525	0.146381	0.000160
C	2.659523	1.249859	0.000173
H	-1.061763	-2.225563	-0.000384
H	-4.585864	0.289861	-0.000638
H	-3.094123	2.257803	-0.000278

H	1.061762	-2.225564	-0.000199
H	4.585866	0.289855	0.000270
H	3.094127	2.257798	0.000300
N	-1.330665	1.189494	-0.000132
N	1.330667	1.189493	0.000032
O	-3.590792	-2.287993	-0.000902
O	3.590790	-2.287995	0.000000
C	-4.995287	-2.237431	0.001146
H	-5.393821	-1.732713	-0.896938
H	-5.353871	-3.275804	0.002849
H	-5.390957	-1.730693	0.899340
C	4.995286	-2.237427	0.000092
H	5.392337	-1.731822	0.898324
H	5.353879	-3.275799	-0.000031
H	5.392432	-1.731573	-0.897958

1d-t

Geometry with 27 atoms:

Thermal correction to Gibbs Free Energy: 0.16618

Total energy: -2082.089425060

Ni	0.000000	1.610156	-0.000003
C	0.715256	-1.023940	0.000058
C	1.531423	-2.184691	0.000374
C	2.900830	-2.058146	0.000347
C	3.490568	-0.768348	0.000031
C	2.656389	0.340332	-0.000137
C	-0.715256	-1.023940	-0.000057
C	-1.531423	-2.184691	-0.000375
C	-2.900830	-2.058146	-0.000348
C	-3.490568	-0.768348	-0.000031
C	-2.656389	0.340332	0.000139
H	1.067267	-3.175293	0.000755
H	4.576113	-0.636426	-0.000037
H	-1.067267	-3.175293	-0.000757
H	-4.576113	-0.636426	0.000038
N	1.315601	0.224566	-0.000099
N	-1.315601	0.224566	0.000101
H	-3.533676	-2.951182	-0.000630
H	3.533676	-2.951182	0.000627
C	3.168154	1.742739	-0.000336
H	2.788817	2.284114	-0.885211
H	2.789153	2.284236	0.884614
H	4.266674	1.792719	-0.000531
C	-3.168154	1.742739	0.000342
H	-2.788828	2.284107	0.885226
H	-2.789142	2.284243	-0.884598
H	-4.266674	1.792719	0.000525

1e-t

Geometry with 23 atoms:

Thermal correction to Gibbs Free Energy: 0.13042

Total energy: -2079.678437830

Ni	0.000001	2.257614	-0.000040
C	0.703282	-0.339094	-0.000043
C	1.435357	-1.566534	-0.000063
C	2.826472	-1.510483	-0.000050
C	3.465105	-0.252565	-0.000086
C	2.686467	0.897310	-0.000111
C	-0.703284	-0.339092	0.000052
C	-1.435357	-1.566533	0.000121
C	-2.826473	-1.510484	0.000107
C	-3.465106	-0.252564	0.000095
C	-2.686470	0.897310	0.000074
H	4.554794	-0.168483	-0.000080
H	-4.554795	-0.168482	0.000088
N	1.347413	0.890888	-0.000072
N	-1.347413	0.890890	0.000033
H	-3.405629	-2.439914	0.000096
H	3.405629	-2.439913	-0.000002
C	0.680341	-2.792475	0.000071
C	-0.680340	-2.792474	0.000037
H	3.163241	1.885325	-0.000129
H	-3.163243	1.885325	0.000053
H	1.236149	-3.736711	0.000157
H	-1.236149	-3.736709	-0.000013

1f-s

Geometry with 27 atoms:

Thermal correction to Gibbs Free Energy: 0.168531

Total energy: -2082.047430480

Ni	0.000002	2.217832	0.000004
C	0.707974	-0.367725	-0.066662
C	1.556059	-1.485539	0.098530
C	2.928790	-1.356886	0.070110
C	3.451010	-0.038390	-0.100049
C	2.593681	1.016547	-0.285019
C	-0.707974	-0.367725	0.066649
C	-1.556061	-1.485539	-0.098539
C	-2.928792	-1.356883	-0.070109
C	-3.451010	-0.038387	0.100051
C	-2.593679	1.016549	0.285016
H	1.104965	-2.463671	0.303748
H	4.532825	0.128961	-0.124154
H	2.982678	2.028103	-0.455927
H	-1.104971	-2.463672	-0.303759
H	-4.532826	0.128964	0.124161
H	-2.982673	2.028107	0.455924
N	1.242313	0.889734	-0.354488

N	-1.242312	0.889733	0.354478
C	3.852908	-2.516884	0.249514
H	4.499842	-2.389377	1.135430
H	3.302607	-3.462677	0.367288
H	4.532924	-2.625897	-0.613780
C	-3.852912	-2.516881	-0.249503
H	-4.499861	-2.389370	-1.135407
H	-3.302614	-3.462673	-0.367290
H	-4.532914	-2.625897	0.613802

1f-t

Geometry with 27 atoms:

Thermal correction to Gibbs Free Energy: 0.167933

Total energy: -2082.080371410

Ni	0.000006	2.310283	-0.000001
C	0.714617	-0.312694	-0.000003
C	1.522249	-1.484101	0.000108
C	2.898225	-1.405101	0.000052
C	3.491040	-0.109055	-0.000116
C	2.663892	0.997649	-0.000169
C	-0.714620	-0.312693	0.000007
C	-1.522254	-1.484099	-0.000080
C	-2.898230	-1.405095	-0.000040
C	-3.491043	-0.109048	0.000087
C	-2.663892	0.997654	0.000126
H	1.043819	-2.469205	0.000284
H	4.578820	0.010988	-0.000179
H	3.092688	2.008161	-0.000265
H	-1.043826	-2.469203	-0.000224
H	-4.578823	0.010996	0.000132
H	-3.092685	2.008168	0.000197
N	1.326333	0.932970	-0.000111
N	-1.326334	0.932972	0.000086
C	3.765152	-2.620437	0.000207
H	4.428852	-2.636494	0.882743
H	3.174637	-3.549344	0.000150
H	4.429110	-2.636537	-0.882132
C	-3.765160	-2.620429	-0.000163
H	-4.428881	-2.636492	-0.882683
H	-3.174649	-3.549339	-0.000109
H	-4.429098	-2.636517	0.882191

1g-t

Geometry with 19 atoms:

Thermal correction to Gibbs Free Energy: 0.105427

Total energy: -2001.532542790

Ni	-1.831701	0.031394	0.000000
N	-0.449283	0.023010	-1.354856
C	0.717639	-0.039790	-0.699330
C	-0.127918	-0.127757	-2.759996
C	1.366813	0.180953	-2.802270
H	-0.338894	-1.157847	-3.118581
H	1.937911	-0.422904	-3.523146
N	-0.449283	0.023010	1.354856
C	-0.127918	-0.127757	2.759996
C	0.717639	-0.039790	0.699330
C	1.366813	0.180953	2.802270
H	-0.706458	0.555733	3.404494
H	1.937911	-0.422904	3.523146
O	1.825555	-0.113389	-1.479962
O	1.825555	-0.113389	1.479962
H	-0.706458	0.555733	-3.404494
H	1.552595	1.251114	-3.017416
H	-0.338894	-1.157847	3.118581
H	1.552595	1.251114	3.017416

1h-t

Geometry with 30 atoms:

Thermal correction to Gibbs Free Energy: 0.182455

Total energy: -2250.501865370

C	-2.728307	0.117350	-1.222786
C	-1.312832	-0.085954	-1.181364
N	-0.713566	-0.273643	-0.000000
C	-1.312832	-0.085954	1.181364
C	-2.728307	0.117350	1.222786
C	-3.400069	0.188252	-0.000000
C	-0.379427	-0.037492	-2.287696
C	-0.379427	-0.037492	2.287696
C	-0.772631	-0.115200	3.639950
C	0.175035	-0.052055	4.641921
C	1.532054	0.098745	4.298960
C	1.855180	0.201637	2.955166
N	0.951945	0.161683	-1.966357
N	0.951945	0.161683	1.966357
C	1.855180	0.201637	-2.955166
C	1.532054	0.098745	-4.298960
C	0.175035	-0.052055	-4.641921
C	-0.772631	-0.115200	-3.639950
Ni	1.290877	-0.145703	0.000000
H	-3.262923	0.240184	-2.168087
H	-3.262923	0.240184	2.168087
H	-4.484596	0.342948	-0.000000
H	-1.830164	-0.255615	3.880394
H	-0.126969	-0.128203	5.690329
H	2.313545	0.157548	5.059337
H	2.896175	0.353487	2.647146
H	2.896175	0.353487	-2.647146
H	2.313545	0.157548	-5.059337

H	-0.126969	-0.128203	-5.690329
H	-1.830164	-0.255615	-3.880394

1a'-s

Geometry with 22 atoms:

Thermal correction to Gibbs Free Energy: 0.118011

Total energy: -4577.656535100

Ni	-0.872046	-0.378224	-0.000345
C	1.925223	-0.404417	0.000026
C	3.235493	-0.880256	0.000402
C	3.457232	-2.253198	0.000341
C	2.362300	-3.114801	-0.000117
C	1.085907	-2.566923	-0.000502
C	1.564058	1.025836	-0.000001
C	2.486938	2.071350	0.000906
C	2.019250	3.381239	0.000715
C	0.645443	3.613215	-0.000349
C	-0.210894	2.518286	-0.001148
H	4.077946	-0.185632	0.000712
H	2.490594	-4.199066	-0.000192
H	0.195245	-3.203728	-0.000860
H	3.559982	1.869008	0.001836
H	0.239178	4.626640	-0.000519
H	-1.299701	2.642346	-0.001927
N	0.867211	-1.246773	-0.000448
N	0.235585	1.260426	-0.001005
H	4.476722	-2.645914	0.000621
H	2.724904	4.215464	0.001412
Br	-3.176939	-0.370469	0.000489

1b'-s

Geometry with 46 atoms:

Thermal correction to Gibbs Free Energy: 0.325871

Total energy: -4892.039928160

Ni	-1.924644	-1.307699	-0.000942
C	0.755995	-0.483888	-0.000813
C	2.144300	-0.538803	-0.000517
C	2.808847	-1.772264	-0.000086
C	2.003444	-2.915876	-0.000311
C	0.620201	-2.787588	-0.001052
C	-0.023140	0.770341	-0.000669
C	0.536728	2.042355	0.000218
C	-0.283788	3.178640	-0.000364
C	-1.664979	2.956384	-0.001465
C	-2.153659	1.655081	-0.001811
H	2.715384	0.393769	-0.000803
H	2.433401	-3.919242	0.000009
H	-0.024403	-3.673406	-0.001661
H	1.624663	2.150458	0.001456
H	-2.378001	3.782994	-0.002010
H	-3.231745	1.456328	-0.002212
N	-0.000912	-1.605654	-0.001251
N	-1.360260	0.585450	-0.001494
C	4.330522	-1.819794	0.000429
C	0.339903	4.567391	0.000483
C	1.209455	4.723131	-1.250160
H	1.662826	5.728958	-1.270971
H	2.030814	3.988511	-1.281945
H	0.610136	4.602980	-2.169045
C	1.206907	4.722444	1.253041
H	1.660118	5.728295	1.275339
H	0.605582	4.601749	2.170552
H	2.028119	3.987731	1.286020
C	-0.716049	5.666268	-0.000303
H	-1.360570	5.620623	-0.894445
H	-1.362202	5.620427	0.892649
H	-0.222497	6.652185	0.000257
C	4.851414	-1.108619	-1.251545
H	4.549372	-0.048967	-1.286165
H	5.954267	-1.140173	-1.271642
H	4.481921	-1.597542	-2.169354
C	4.850672	-1.107221	1.251956
H	4.480258	-1.594860	2.170079
H	5.953498	-1.139269	1.272992
H	4.549046	-0.047419	1.284972
C	4.854925	-3.250742	0.001417
H	4.530289	-3.810002	0.895214
H	4.530891	-3.811040	-0.891942
H	5.957450	-3.239934	0.001762
Br	-4.068302	-2.100560	0.001308

1c'-s

Geometry with 30 atoms:

Thermal correction to Gibbs Free Energy: 0.176149

Total energy: -4806.682639010

Ni	-0.995722	-1.331995	0.000019
C	0.203152	1.224141	-0.000011
C	0.367970	2.599133	-0.000007
C	-0.766586	3.423916	-0.000024
C	-2.032023	2.821024	-0.000041
C	-2.095683	1.434252	-0.000044
C	1.321844	0.258200	0.000013
C	2.655980	0.629192	-0.000013
C	3.645698	-0.364459	0.000013
C	3.241372	-1.706005	0.000066
C	1.881411	-1.981718	0.000087
H	1.357710	3.062036	0.000011
H	-2.955885	3.402166	-0.000053

H	-3.065040	0.922323	-0.000061
H	2.960302	1.678825	-0.000056
H	3.955846	-2.531073	0.000089
H	1.531525	-3.019737	0.000129
N	-1.019621	0.648479	-0.000031
N	0.934039	-1.040267	0.000063
O	-0.550841	4.737309	-0.000024
O	4.911209	0.047931	-0.000014
C	-1.660328	5.613036	0.000002
H	-2.284076	5.474490	0.899607
H	-1.258303	6.634093	0.000031
H	-2.284079	5.474541	-0.899608
C	5.944163	-0.916625	0.000000
H	5.901545	-1.554035	-0.899635
H	6.892779	-0.364997	-0.000030
H	5.901571	-1.553981	0.899675
Br	-2.837125	-2.687791	-0.000023

1d'-s

Geometry with 28 atoms:

Thermal correction to Gibbs Free Energy: 0.16647

Total energy: -4656.271151830

Ni	-0.815360	-0.000010	0.000003
C	1.903187	0.737947	-0.003816
C	3.060192	1.513681	-0.024528
C	2.931357	2.898262	-0.028003
C	1.661363	3.464131	-0.010808
C	0.539374	2.632704	0.007070
C	1.903201	-0.737917	0.003812
C	3.060219	-1.513632	0.024515
C	2.931407	-2.898215	0.027995
C	1.661422	-3.464105	0.010811
C	0.539419	-2.632698	-0.007059
H	4.047437	1.047467	-0.041496
H	1.525376	4.548785	-0.012441
H	4.047456	-1.047401	0.041473
H	1.525455	-4.548761	0.012449
N	0.674304	1.295110	0.008932
N	0.674327	-1.295101	-0.008925
H	3.821052	-3.533322	0.044599
H	3.820991	3.533385	-0.044614
C	-0.849706	3.165228	0.031923
H	-1.441036	2.732822	-0.792180
H	-1.360118	2.862948	0.962180
H	-0.867674	4.261630	-0.042115
C	-0.849652	-3.165246	-0.031904
H	-1.440996	-2.732821	0.792180
H	-1.360062	-2.863007	-0.962176
H	-0.867603	-4.261645	0.042170
Br	-3.114609	-0.000020	-0.000007

1e'-s

Geometry with 24 atoms:

Thermal correction to Gibbs Free Energy: 0.130582

Total energy: -4653.856698330

Ni	-1.263136	-0.388124	0.000023
C	1.260310	0.800335	0.000006
C	2.342619	1.702239	-0.000013
C	2.027036	3.077097	-0.000008
C	0.702142	3.467833	0.000018
C	-0.304830	2.487914	0.000036
C	1.498982	-0.611600	0.000014
C	2.819332	-1.102844	-0.000015
C	2.982816	-2.503911	-0.000016
C	1.862538	-3.312020	0.000010
C	0.587137	-2.726116	0.000038
H	0.425503	4.524079	0.000028
H	1.951506	-4.400308	0.000006
N	-0.035874	1.191266	0.000031
N	0.400978	-1.410771	0.000037
H	3.989665	-2.931330	-0.000048
H	2.833260	3.816615	-0.000014
Br	-3.551886	-0.088707	-0.000030
C	3.677777	1.178692	-0.000010
C	3.905386	-0.165330	-0.000066
H	4.512594	1.885506	-0.000017
H	4.926538	-0.557682	-0.000097
H	-1.364849	2.766439	0.000052
H	-0.313611	-3.348326	0.000062

1f'-s

Geometry with 28 atoms:

Thermal correction to Gibbs Free Energy: 0.166192

Total energy: -4656.260317440

Ni	1.299912	-0.414322	0.000242
Br	3.585325	-0.447415	0.001342
C	-1.501770	-0.513398	-0.001011
C	-2.799498	-1.020215	-0.002837
C	-3.012581	-2.400202	-0.003348
C	-1.877847	-3.222645	-0.003756
C	-0.616444	-2.650090	-0.001663
C	-1.176230	0.926249	-0.001082
C	-2.124424	1.947599	-0.002791
C	-1.711094	3.281635	-0.003363
C	-0.331386	3.528415	-0.003841
C	0.553143	2.461589	-0.001868
H	-3.656257	-0.340150	-0.004976
H	-1.981592	-4.311734	-0.006733

H	0.286111	-3.270945	-0.002240
H	-3.192574	1.712657	-0.004647
H	0.048704	4.554287	-0.006762
H	1.637904	2.619361	-0.002459
N	-0.421615	-1.325243	-0.000100
N	0.145486	1.189254	-0.000378
C	-4.384008	-2.984024	0.004907
H	-4.572799	-3.519342	0.950883
H	-5.158903	-2.212532	-0.110598
H	-4.502283	-3.724731	-0.802576
C	-2.690442	4.405572	0.004587
H	-2.476755	5.120304	-0.806635
H	-3.724749	4.049241	-0.105316
H	-2.622306	4.973132	0.948067

1g'-s

Geometry with 20 atoms:

Thermal correction to Gibbs Free Energy: 0.101193

Total energy: -4575.704207320

Ni	-0.828276	-0.181625	-0.000015
N	0.551735	1.299769	0.000086
C	1.747124	0.831735	0.000058
C	0.677451	2.752841	0.000035
C	2.194846	2.995522	0.000056
H	0.176550	3.174795	-0.886152
H	2.560175	3.521637	-0.894010
N	0.797358	-1.304437	-0.000019
C	1.196607	-2.709000	0.000041
C	1.885122	-0.618413	0.000056
C	2.732148	-2.660082	0.000114
H	0.784023	-3.216957	0.886395
H	3.189673	-3.108325	-0.893941
O	2.773183	1.662465	0.000018
O	3.048596	-1.242766	0.000143
H	0.176520	3.174872	0.886168
H	2.560153	3.521572	0.894169
H	0.784113	-3.217017	-0.886320
H	3.189593	-3.108345	0.894200
Br	-3.109907	-0.072493	-0.000115

1h'-s

Geometry with 31 atoms:

Thermal correction to Gibbs Free Energy: 0.180881

Total energy: -4824.664297970

C	-1.206273	3.359862	0.126447
C	-1.175309	1.970919	0.198339
N	0.000326	1.308563	0.369796
C	1.176249	1.970429	0.198326
C	1.207790	3.359369	0.126421
C	0.000911	4.066750	0.137709
C	-2.316767	1.086251	-0.003916
C	2.317354	1.085324	-0.003905
C	3.657924	1.470568	0.135194
C	4.657218	0.550253	-0.131883
C	4.305797	-0.749675	-0.522094
C	2.962282	-1.069515	-0.617309
N	-1.986416	-0.181045	-0.379444
N	1.986536	-0.181837	-0.379563
C	-2.962487	-1.068307	-0.617349
C	-4.305892	-0.747928	-0.522238
C	-4.656826	0.552111	-0.131994
C	-3.657180	1.472023	0.135171
Ni	0.000173	-0.634332	0.027103
H	-2.157340	3.886591	0.011860
H	2.159076	3.885698	0.011808
H	0.001134	5.156872	0.068639
H	3.902655	2.483188	0.465547
H	5.707788	0.833667	-0.028780
H	5.065427	-1.501657	-0.744934
H	2.632399	-2.078047	-0.892467
H	-2.632975	-2.076963	-0.892505
H	-5.065804	-1.499592	-0.745190
H	-5.707291	0.835943	-0.028977
H	-3.901526	2.484738	0.465519
Br	-0.001151	-3.003415	0.378102

2

Geometry with 15 atoms:

Thermal correction to Gibbs Free Energy: 0.082834

Total energy: -2844.909792210

C	-1.735503	1.200458	-0.010693
C	-0.342715	1.211538	-0.004830
C	0.344721	0.000094	-0.000710
C	-0.342908	-1.211354	-0.004823
C	-1.735583	-1.200084	-0.010712
C	-2.456559	0.000273	-0.010393
H	-2.277236	2.152729	-0.017826
H	0.203053	2.159524	-0.006857
H	0.202793	-2.159382	-0.006841
H	-2.277508	-2.152261	-0.017862
Br	2.243922	-0.000084	0.003343
C	-3.952132	-0.000198	0.014814
H	-4.331359	-0.012504	1.051931
H	-4.366701	0.898485	-0.467597
H	-4.366238	-0.887997	-0.487880

CP-1a-t

Geometry with 36 atoms:

Thermal correction to Gibbs Free Energy: 0.222718

Total energy: -4848.432399570

C	2.263184	1.082397	-0.983275
C	2.163073	-0.101310	-0.214716
C	1.966306	-0.023379	1.185419
C	1.840107	1.252615	1.783327
C	1.933872	2.426708	1.034037
C	2.152109	2.317148	-0.356564
Br	2.572668	-1.770250	-1.031800
H	2.003819	-0.921052	1.810532
H	2.438319	1.020668	-2.061051
H	2.221565	3.228845	-0.959704
H	1.688081	1.313166	2.865892
C	-2.296478	-1.018946	0.207503
C	-0.631813	-2.513385	0.923030
C	-1.535516	-3.542493	1.110085
C	-2.900242	-3.281394	0.827804
C	-3.273036	-2.035923	0.382857
C	-2.573772	0.305739	-0.247590
C	-1.651844	2.410103	-0.765916
C	-2.878802	2.940901	-1.110516
C	-4.015351	2.095138	-1.015132
C	-3.861558	0.797391	-0.591298
H	0.435243	-2.672619	1.129114
H	-1.196688	-4.518946	1.463862
H	-4.322740	-1.821855	0.162784
H	-0.740401	3.021029	-0.828545
H	-2.958940	3.976973	-1.447319
H	-4.729969	0.136701	-0.517133
N	-0.970343	-1.292437	0.491702
N	-1.480236	1.148207	-0.346183
Ni	0.180571	0.289588	0.190759
C	1.760108	3.770034	1.662023
H	-5.008318	2.471596	-1.279112
H	-3.653339	-4.063813	0.962619
H	2.519858	4.482893	1.302996
H	0.775893	4.199358	1.402499
H	1.820204	3.718898	2.759228

CP-1b-t

Geometry with 60 atoms:

Thermal correction to Gibbs Free Energy: 0.42949

Total energy: -5162.811080990

C	-3.260596	-0.807852	1.161395
C	-3.301839	-0.961670	-0.248308
C	-3.779876	0.089235	-1.066028
C	-4.196215	1.266196	-0.479370
C	-4.160509	1.454151	0.923679
C	-3.687718	0.420684	1.717385
Br	-3.112919	-2.717398	-1.009142
H	-3.829778	-0.042755	-2.150884
H	-3.084518	-1.669468	1.816688
H	-3.672903	0.537457	2.806317
H	-4.561450	2.080393	-1.115191
C	1.423704	-0.499101	0.149992
C	0.714609	-2.711448	0.434423
C	2.006561	-3.197988	0.424698
C	3.088249	-2.285140	0.265002
C	2.767302	-0.947293	0.131029
C	1.005967	0.862052	0.027171
C	-0.806201	2.333027	-0.027699
C	0.008540	3.432648	-0.184484
C	1.424697	3.252457	-0.242824
C	1.891803	1.959936	-0.135469
H	-0.131357	-3.400661	0.556453
H	2.167025	-4.271302	0.539227
H	3.563354	-0.206978	0.005173
H	-1.894891	2.461229	0.014210
H	-0.444926	4.424526	-0.263672
H	2.964220	1.755563	-0.173736
N	0.401637	-1.416252	0.300571
N	-0.359346	1.072289	0.079229
Ni	-1.370366	-0.617613	0.286307
C	-4.601169	2.756795	1.507507
C	2.331672	4.462590	-0.416466
C	4.547064	-2.735575	0.227787
C	5.334618	-2.018304	1.327113
H	6.388816	-2.346645	1.319928
H	5.328700	-0.923774	1.196373
H	4.918547	-2.241930	2.324907
C	4.685754	-4.239186	0.442870
H	4.171441	-4.819679	-0.341619
H	5.751504	-4.522389	0.415501
H	4.285069	-4.555745	1.420959
C	5.145503	-2.386245	-1.137635
H	6.198271	-2.715229	-1.192340
H	4.593010	-2.885625	-1.952582
H	5.124402	-1.301035	-1.331584
C	3.805783	4.078366	-0.460262
H	4.423855	4.982841	-0.588921
H	4.132486	3.585616	0.471287
H	4.031574	3.401859	-1.302073
C	2.115713	5.423318	0.756508
H	2.364011	4.938251	1.716665
H	2.762591	6.311567	0.649303
H	1.073507	5.777716	0.817187
C	1.976398	5.171823	-1.726580
H	2.122399	4.501923	-2.591901

H	0.929916	5.518467	-1.741204
H	2.621008	6.056400	-1.871292
H	-3.918068	3.572689	1.211266
H	-5.602884	3.041344	1.144953
H	-4.627445	2.724347	2.606786

CP-1c-t

Geometry with 44 atoms:

Thermal correction to Gibbs Free Energy: 0.279603

Total energy: -5077.449145890

C	2.671419	-0.970165	-1.009327
C	2.213504	-1.598348	0.178126
C	2.561849	-1.074892	1.446587
C	3.328629	0.068509	1.513798
C	3.822030	0.706568	0.349503
C	3.493874	0.172951	-0.886729
Br	1.540431	-3.404043	0.069524
H	2.221116	-1.576395	2.357241
H	2.583066	-1.470848	-1.980006
H	3.884745	0.639715	-1.797769
H	3.577316	0.488652	2.494577
C	-1.987205	0.296530	-0.080849
C	-2.006895	-2.030480	-0.352085
C	-3.368356	-2.131797	-0.120432
C	-4.073877	-0.928210	0.152705
C	-3.385041	0.269798	0.170864
C	-1.190073	1.475481	-0.109373
C	0.934668	2.369268	-0.494186
C	0.511685	3.677216	-0.317244
C	-0.857017	3.881596	0.001824
C	-1.695962	2.787168	0.094326
H	-1.429687	-2.940281	-0.562367
H	-3.852650	-3.108508	-0.150847
H	-3.939174	1.188102	0.383021
H	1.984234	2.182238	-0.750260
H	1.223995	4.495524	-0.431201
H	-2.752229	2.955157	0.320673
N	-1.317927	-0.889073	-0.342680
N	0.159164	1.291745	-0.380067
Ni	0.613719	-0.641647	-0.512078
C	4.643009	1.948290	0.476626
O	-1.397438	5.093801	0.211825
O	-5.394250	-0.883920	0.398788
C	-0.577041	6.232676	0.117153
H	-1.211767	7.103442	0.330477
H	0.246427	6.211328	0.852665
H	-0.149394	6.351070	-0.894158
C	-6.131974	-2.081849	0.393989
H	-7.174670	-1.816450	0.615325
H	-6.100233	-2.583480	-0.589374
H	-5.779187	-2.787610	1.166722
H	4.042374	2.771529	0.903628
H	5.498492	1.800930	1.156733
H	5.029512	2.283904	-0.497551

CP-1d-t

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.275518

Total energy: -4927.036102150

C	2.528923	0.320140	0.125875
C	2.082727	-1.765194	1.128729
C	3.418003	-2.134438	1.037390
C	4.337573	-1.253890	0.423402
C	3.896365	-0.030969	-0.015401
C	2.017456	1.613168	-0.202241
C	0.113868	3.019223	-0.165688
C	0.857478	4.106468	-0.599232
C	2.233759	3.923792	-0.876948
C	2.807596	2.691794	-0.678317
H	3.738971	-3.097586	1.443297
H	4.595438	0.678785	-0.464921
H	0.374241	5.079122	-0.724780
H	3.873086	2.544963	-0.871997
N	1.621879	-0.588893	0.647557
N	0.666126	1.801020	0.017312
Ni	-0.256197	0.117162	0.383777
H	-2.889390	-0.408739	2.599631
C	-2.755784	-0.342690	1.514445
C	-1.808292	-1.198803	0.899379
C	-3.544463	0.528428	0.778563
C	-1.638256	-1.124175	-0.507374
H	-1.373074	-2.013612	1.481256
C	-3.382478	0.550058	-0.627523
C	-2.456626	-0.247541	-1.265806
H	-4.007430	1.224955	-1.223319
H	-2.358138	-0.221430	-2.355001
Br	-0.730628	-2.508422	-1.469416
C	-4.541391	1.434380	1.422892
H	-4.295104	2.493541	1.230318
H	-5.552829	1.271276	1.013818
H	-4.583874	1.288171	2.512408
H	2.839952	4.761112	-1.236056
H	5.390111	-1.534059	0.318722
C	-1.345450	3.136038	0.110209
H	-1.930741	2.675824	-0.705212
H	-1.607396	2.594277	1.035480
H	-1.662556	4.184939	0.203168
C	1.113812	-2.679709	1.802601

H	0.519642	-2.135683	2.555281
H	0.411574	-3.129266	1.080609
H	1.638063	-3.503723	2.307307

CP-1e-t

Geometry with 38 atoms:

Thermal correction to Gibbs Free Energy: 0.235063

Total energy: -4924.630352560

C	-2.332527	-0.154274	1.188608
C	-2.411596	-0.492569	-0.186927
C	-2.777335	0.484681	-1.141753
C	-3.046191	1.771100	-0.722375
C	-2.970945	2.142592	0.641990
C	-2.608935	1.179034	1.570582
Br	-2.425385	-2.346474	-0.698553
H	-2.857369	0.212969	-2.198346
H	-2.247058	-0.933015	1.956026
H	-2.566824	1.439786	2.633521
H	-3.324341	2.528123	-1.464086
C	2.317666	-0.467802	0.145856
C	1.480722	-2.578314	0.682064
C	2.754054	-3.126204	0.720100
C	3.866341	-2.299656	0.456708
C	3.658266	-0.953348	0.165728
C	2.038476	0.879682	-0.135462
C	0.437023	2.547066	-0.396682
C	1.405590	3.500976	-0.677800
C	2.761783	3.121777	-0.685909
C	3.094676	1.797236	-0.412989
H	2.878986	-4.186529	0.952831
H	1.102590	4.529562	-0.888207
N	1.237931	-1.289309	0.403319
N	0.710171	1.263453	-0.127127
Ni	-0.446975	-0.306753	0.295460
C	-3.259002	3.553015	1.041692
H	3.552963	3.847238	-0.901730
H	4.885662	-2.698804	0.478747
C	4.442248	1.292696	-0.391634
C	4.710644	-0.013283	-0.116580
H	5.743504	-0.377947	-0.104046
H	5.256176	1.994485	-0.603900
H	-0.622674	2.829080	-0.388980
H	0.601674	-3.202754	0.885531
H	-2.513243	4.245847	0.613337
H	-4.242216	3.882956	0.666715
H	-3.246519	3.679231	2.134424

CP-1f-t

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.271127

Total energy: -4927.032859490

C	-2.337292	-0.490826	1.193831
C	-2.427507	-0.711948	-0.204491
C	-2.920116	0.304740	-1.055661
C	-3.301080	1.514927	-0.513517
C	-3.213433	1.770680	0.876114
C	-2.727832	0.769412	1.703276
Br	-2.280138	-2.502759	-0.885695
H	-3.009435	0.121110	-2.130410
H	-2.146619	-1.321859	1.883862
H	-2.673494	0.938739	2.784002
H	-3.678411	2.302029	-1.175855
C	2.318088	-0.278211	0.119826
C	1.575253	-2.456931	0.577203
C	2.858804	-2.955980	0.620887
C	3.950517	-2.064403	0.400199
C	3.660468	-0.739815	0.153756
C	1.918334	1.071503	-0.121403
C	0.115754	2.549673	-0.327646
C	0.941615	3.626457	-0.571200
C	2.351783	3.422477	-0.591437
C	2.815089	2.144249	-0.367036
H	0.715250	-3.118848	0.745116
H	3.034412	-4.017064	0.821771
H	4.478893	-0.032807	-0.017772
H	-0.973084	2.684866	-0.313165
H	0.516167	4.619198	-0.746652
H	3.893124	1.952437	-0.377391
N	1.285057	-1.169408	0.334062
N	0.554971	1.302074	-0.103116
Ni	-0.474905	-0.350293	0.261595
C	3.268837	4.570437	-0.850599
H	4.326044	4.264895	-0.840420
H	3.055114	5.036827	-1.828333
H	3.133567	5.365140	-0.096026
C	5.350311	-2.579058	0.441410
H	6.088436	-1.783276	0.259584
H	5.575452	-3.040221	1.419108
H	5.504850	-3.370300	-0.313164
C	-3.610695	3.108464	1.409360
H	-2.911642	3.891601	1.065515
H	-4.611075	3.403360	1.051715
H	-3.616945	3.125181	2.509318

CP-1g-t

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.20963

Total energy: -4846.484803790

C	-1.878725	-0.132461	1.195615
C	-1.879555	-0.665558	-0.122111
C	-2.254603	0.146083	-1.220742
C	-2.593756	1.463755	-1.000787
C	-2.608974	2.025416	0.301410
C	-2.255096	1.222062	1.371491
Br	-1.787335	-2.577818	-0.353867
H	-2.272116	-0.275384	-2.230290
H	-1.810896	-0.791540	2.069018
H	-2.287834	1.629600	2.388005
H	-2.866889	2.095187	-1.853906
C	-3.008345	3.453692	0.486208
H	-2.391677	4.125661	-0.135375
H	-4.054728	3.619894	0.176972
H	-2.910348	3.772561	1.534797
Ni	0.021314	-0.318978	0.352794
N	0.917988	1.413216	-0.072888
C	2.230805	1.209283	-0.162512
C	0.715743	2.842991	-0.185534
C	2.060441	3.345379	-0.715986
H	-0.113039	3.095005	-0.871520
H	2.043753	3.477237	-1.813776
N	1.832075	-1.052610	0.322079
C	2.561208	-2.304417	0.274472
C	2.710713	-0.095908	0.014051
C	4.016966	-1.847957	0.355099
H	2.294255	-2.981457	1.102894
H	4.714037	-2.433008	-0.262213
O	2.989494	2.301950	-0.393085
O	3.992437	-0.496425	-0.125994
H	0.459374	3.295237	0.795931
H	2.406496	4.284246	-0.259092
H	2.356054	-2.854616	-0.667689
H	4.386649	-1.846201	1.397618
C	-3.727767	-0.708600	-1.940515
C	-2.368027	-0.967280	-1.840933
N	2.359358	-0.014132	-0.684622
N	-1.476732	-0.058568	-1.422940
C	3.385236	-0.880914	-0.720887
C	4.677390	-0.572732	-0.340228
C	4.943331	0.741316	0.119689
C	3.912443	1.651378	0.172279
Ni	0.452095	-0.312375	-1.049632
H	2.236467	3.985072	0.699427
H	-2.030582	3.860641	-0.040896
H	0.020964	5.086882	0.743363
H	-3.608023	2.513480	-0.867067
H	-5.256550	0.801825	-1.647460
H	-4.407693	-1.489200	-2.288341
H	-1.964738	-1.953685	-2.098576
H	3.140087	-1.889546	-1.077941
H	5.462531	-1.329905	-0.398396
H	5.951744	1.029292	0.430142
H	4.089296	2.672352	0.524598
C	-0.497918	-1.830506	1.196088
C	0.274985	-0.803816	1.733638
C	-1.887333	-1.805674	1.280348
C	-0.367392	0.280782	2.329759
H	1.366403	-0.849191	1.693224
C	-2.507558	-0.705204	1.864792
H	-2.482377	-2.620978	0.858653
C	-1.761913	0.363314	2.381756
H	0.237657	1.100277	2.734137
H	-3.602176	-0.665310	1.902275
Br	0.355346	-3.249125	0.256879
C	-2.451417	1.554182	2.970427
H	-2.897364	1.320006	3.952105
H	-1.756794	2.396182	3.110023
H	-3.274574	1.894041	2.320016

CP-1h-t

Geometry with 45 atoms:

Thermal correction to Gibbs Free Energy: 0.286021

Total energy: -5095.455999250

C	1.356988	3.461376	0.312233
C	1.465867	2.148304	-0.195779
N	0.340095	1.556517	-0.685439
C	-0.874670	2.112242	-0.613514
C	-1.045496	3.392307	-0.109475
C	0.114202	4.073525	0.343112
C	2.608244	1.280132	-0.228625
C	-1.924604	1.182056	-1.076916
C	-3.278278	1.511032	-1.151612
C	-4.192835	0.558933	-1.585530

CP'-1a-t

Geometry with 36 atoms:

Thermal correction to Gibbs Free Energy: 0.220298

Total energy: -4848.424182580

Ni	-0.708703	-0.861618	-0.362519
C	2.629346	-0.623803	-0.152021
C	3.983774	-0.867593	-0.338698
C	2.160801	0.328020	0.744331
C	4.894294	-0.123111	0.407753
H	4.333464	-1.618819	-1.052987
C	3.092671	1.057348	1.477982
H	1.083644	0.499967	0.856139
C	4.468523	0.844672	1.326615

H	5.966543	-0.299045	0.269422
H	2.738638	1.814932	2.185287
Br	1.350335	-1.629645	-1.180926
N	-2.437922	-0.947522	0.451741
C	-4.995803	-0.723095	1.547476
C	-3.046849	-2.009616	1.002411
C	-3.092311	0.273915	0.428651
C	-4.392586	0.378250	0.988353
C	-4.309078	-1.964664	1.560333
N	-1.123821	1.023338	-0.678765
C	-2.075098	3.637169	-0.914095
C	-0.388090	1.972791	-1.273298
C	-2.373565	1.348725	-0.180051
C	-2.849292	2.680841	-0.301355
C	-0.799083	3.282857	-1.423096
H	-2.475764	-2.946358	0.988380
H	-4.912620	1.340388	0.970214
H	-4.753118	-2.863115	1.995251
H	0.593503	1.654539	-1.650802
H	-3.834081	2.942168	0.096279
H	-0.154220	4.012164	-1.918806
C	5.458287	1.613546	2.141715
H	-2.442586	4.663697	-1.006736
H	-5.998482	-0.640336	1.977693
H	6.400251	1.770092	1.593746
H	5.060853	2.594861	2.442638
H	5.712494	1.069510	3.068347

CP'-1b-t

Geometry with 60 atoms:

Thermal correction to Gibbs Free Energy: 0.426206

Total energy: -5162.802371720

Ni	0.704716	-1.255114	-0.834557
C	3.942127	-0.896543	-0.060533
C	5.323532	-1.037546	-0.071416
C	3.269695	-0.232291	0.957252
C	6.048454	-0.486967	0.983506
H	5.835741	-1.561893	-0.883605
C	4.018445	0.307632	1.999291
H	2.178109	-0.133494	0.925627
C	5.413592	0.188781	2.033223
H	7.139347	-0.585025	0.988243
H	3.502888	0.838672	2.806658
Br	2.914787	-1.634225	-1.513100
N	-1.089277	-1.661591	-0.310611
C	-3.800500	-1.887389	0.462144
C	-1.665280	-2.857106	-0.131932
C	-1.853156	-0.521959	-0.109868
C	-3.210531	-0.651411	0.277678
C	-2.982871	-3.033971	0.244505
N	0.147236	0.615366	-0.712918
C	-1.044693	3.159699	-0.397458
C	0.836140	1.738791	-0.936358
C	-1.177223	0.719072	-0.322946
C	-1.762095	2.001262	-0.166566
C	0.313705	3.011309	-0.801156
H	-1.020900	-3.728589	-0.303822
H	-3.797543	0.259869	0.430592
H	-3.364615	-4.049043	0.366614
H	1.882987	1.608883	-1.244951
H	-2.809611	2.062776	0.145436
H	0.954803	3.869973	-1.007642
C	6.202414	0.747773	3.173740
H	7.219952	1.030810	2.863418
H	5.711468	1.630340	3.611813
H	6.307279	0.003211	3.982388
C	-5.266437	-1.987985	0.879455
C	-5.719334	-3.436759	1.029277
H	-5.141738	-3.973571	1.800938
H	-6.779750	-3.466317	1.331879
H	-5.631112	-3.998290	0.083684
C	-6.143942	-1.316800	-0.180494
H	-7.209917	-1.391465	0.098244
H	-5.905581	-0.246788	-0.298129
H	-6.017897	-1.800719	-1.164746
C	-5.462165	-1.281217	2.223300
H	-4.836472	-1.740551	3.008372
H	-5.203311	-0.210870	2.169253
H	-6.515704	-1.352893	2.546508
C	-1.706255	4.524785	-0.217985
C	-2.902787	4.638046	-1.166170
H	-3.665725	3.868551	-0.962906
H	-3.387716	5.624369	-1.058681
H	-2.586865	4.530311	-2.218508
C	-2.187460	4.669870	1.228099
H	-2.659263	5.656707	1.380053
H	-2.931111	3.901228	1.495718
H	-1.345358	4.585942	1.937084
C	-0.744979	5.669858	-0.520114
H	0.132363	5.661562	0.148826
H	-0.381481	5.641916	-1.561396
H	-1.258969	6.635399	-0.376998

CP'-1c-t

Geometry with 44 atoms:

Thermal correction to Gibbs Free Energy: 0.276206

Total energy: -5077.442294930

Ni	-0.030805	-1.014166	-0.723936

C	3.265514	-0.916706	-0.137060
C	4.629175	-1.161254	-0.232634
C	2.710063	-0.196511	0.912894
C	5.458282	-0.660451	0.768602
H	5.048338	-1.727018	-1.069949
C	3.561626	0.292259	1.899932
H	1.629388	-0.014499	0.948636
C	4.943181	0.068102	1.848314
H	6.536950	-0.840288	0.706588
H	3.139145	0.866253	2.731601
Br	2.099274	-1.588393	-1.513640
N	-1.831946	-1.266852	-0.114357
C	-4.490403	-1.267139	0.766528
C	-2.487327	-2.406463	0.105826
C	-2.487637	-0.060918	0.099471
C	-3.836043	-0.069340	0.546039
C	-3.800875	-2.489067	0.541293
N	-0.427606	0.902554	-0.601985
C	-1.380639	3.516451	-0.286379
C	0.340417	1.955242	-0.871390
C	-1.725201	1.113702	-0.159823
C	-2.202847	2.442321	0.000576
C	-0.055962	3.278011	-0.742232
H	-1.921906	-3.328454	-0.079662
H	-4.377909	0.864149	0.721553
H	-4.260558	-3.465747	0.697381
H	1.359540	1.733738	-1.218248
H	-3.219741	2.639598	0.351108
H	0.640537	4.080764	-0.987440
C	5.842846	0.572521	2.930710
H	6.851736	0.793430	2.549634
H	5.439549	1.481786	3.402152
H	5.958362	-0.180880	3.729666
O	-5.765482	-1.203887	1.188564
O	-1.893102	4.747433	-0.112831
C	-1.088793	5.867337	-0.389584
H	-1.695522	6.758152	-0.177352
H	-0.187920	5.897679	0.248719
H	-0.776797	5.901297	-1.448502
C	-6.470197	-2.399538	1.415623
H	-6.000834	-3.013414	2.204705
H	-7.478989	-2.118746	1.747590
H	-6.560959	-3.007017	0.497726

CP'-1d-t

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.272565

Total energy: -4927.034830420

Ni	-0.565309	0.001353	-0.877617
C	2.702872	-0.012858	-0.344727
C	4.085147	0.027344	-0.476786
C	2.080802	-0.058096	0.898275
C	4.860764	0.025260	0.680726
H	4.554528	0.056988	-1.463930
C	2.879176	-0.059142	2.038479
H	0.984462	-0.096144	0.963170
C	4.276152	-0.013673	1.952607
H	5.951783	0.052633	0.590984
H	2.401357	-0.099096	3.023107
Br	1.614157	-0.011974	-1.926689
N	-1.748693	-1.300151	-0.070569
C	-3.685009	-2.881999	1.156290
C	-1.640673	-2.644085	-0.100372
C	-2.810406	-0.703994	0.585019
C	-3.797654	-1.512362	1.201186
C	-2.578565	-3.471915	0.495640
N	-1.737646	1.311112	-0.073416
C	-3.658913	2.913588	1.148480
C	-1.615652	2.653645	-0.105083
C	-2.804521	0.726084	0.583104
C	-3.784741	1.545143	1.196439
C	-2.545998	3.491766	0.488313
H	-4.643008	-1.043705	1.712526
H	-2.456017	-4.557167	0.449212
H	-4.635070	1.085847	1.707999
H	-2.412613	4.575682	0.440591
C	5.119825	0.016376	3.188420
H	5.279373	1.053026	3.531588
H	4.641764	-0.526440	4.017709
H	6.113613	-0.421603	3.011919
C	-0.440228	-3.178640	-0.809650
H	-0.416124	-2.815758	-1.851804
H	0.482713	-2.809563	-0.328443
H	-0.415674	-4.277451	-0.817731
C	-0.407715	3.173305	-0.812701
H	0.509224	2.793409	-0.328014
H	-0.385969	2.807833	-1.854048
H	-0.370135	4.271734	-0.822738
H	-4.443078	-3.512116	1.630682
H	-4.411597	3.551881	1.620528

CP'-1e-t

Geometry with 38 atoms:

Thermal correction to Gibbs Free Energy: 0.232195

Total energy: -4924.623427400

Ni	-0.319348	-1.114725	-0.328419
C	2.971783	-0.491573	-0.097015
C	4.347186	-0.583426	-0.266928

C	2.387453	0.440284	0.751090
C	5.157812	0.296844	0.446372
H	4.788507	-1.321235	-0.943613
C	3.221076	1.307609	1.452063
H	1.296885	0.490524	0.851367
C	4.613741	1.250485	1.316161
H	6.244421	0.241233	0.320399
H	2.774724	2.051136	2.121065
Br	1.829362	-1.688457	-1.080399
N	-2.069174	-1.314662	0.442512
C	-4.703657	-1.101053	1.425507
C	-2.674044	-2.349174	1.045248
C	-2.782170	-0.133819	0.314686
C	-4.115297	-0.001298	0.806136
C	-3.966927	-2.298163	1.545223
N	-0.851470	0.728593	-0.775811
C	-2.114892	3.221352	-1.133384
C	-0.227996	1.742066	-1.388226
C	-2.140204	0.941377	-0.322666
C	-2.802492	2.194264	-0.491820
C	-0.801366	2.990184	-1.590738
H	-4.395173	-3.181613	2.025146
H	-0.232112	3.771364	-2.100430
C	5.499027	2.167659	2.097464
H	-2.600795	4.192329	-1.275629
H	-5.725818	-1.024245	1.810580
C	-4.768103	1.269545	0.628103
C	-4.145060	2.312031	0.013225
H	-4.659490	3.271094	-0.112252
H	-5.791124	1.377871	1.004844
H	-2.083895	-3.269622	1.129783
H	0.794114	1.542548	-1.737890
H	6.428027	2.395972	1.552658
H	4.991391	3.114605	2.336748
H	5.793703	1.707644	3.057050

CP'-1f-t

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.269681

Total energy: -4927.026375520

Ni	-0.271158	-0.960939	-0.554968
C	3.043255	-0.620468	-0.156480
C	4.410917	-0.821258	-0.285916
C	2.500301	0.196587	0.827322
C	5.258018	-0.173635	0.611089
H	4.819575	-1.465729	-1.069913
C	3.369332	0.831412	1.710039
H	1.414856	0.338347	0.891996
C	4.756437	0.656713	1.621059
H	6.340012	-0.317654	0.520425
H	2.956964	1.483062	2.487897
Br	1.850945	-1.494879	-1.389827
N	-2.025618	-1.265284	0.148216
C	-4.669399	-1.345195	1.113947
C	-2.593101	-2.423754	0.517278
C	-2.762012	-0.096902	0.249549
C	-4.095076	-0.150342	0.737373
C	-3.881594	-2.528017	0.998116
N	-0.799217	0.921608	-0.625897
C	-1.936440	3.495839	-0.552800
C	-0.110392	1.994047	-1.037615
C	-2.090726	1.094933	-0.162855
C	-2.654793	2.398853	-0.128155
C	-0.609632	3.280196	-1.028313
H	-1.963655	-3.316873	0.415652
H	-4.677215	0.774067	0.813456
H	-4.288730	-3.502426	1.284562
H	0.910140	1.800953	-1.396806
H	-3.675827	2.535487	0.243725
H	0.003044	4.116023	-1.379447
C	-2.501905	4.876629	-0.527077
H	-3.531871	4.894269	-0.139656
H	-1.887446	5.546293	0.100074
H	-2.507192	5.322573	-1.537230
C	-6.067339	-1.429805	1.629129
H	-6.555402	-0.443944	1.663886
H	-6.683485	-2.096100	1.000050
H	-6.090821	-1.860507	2.645661
C	5.674668	1.322043	2.595578
H	6.678190	1.473558	2.169648
H	5.281337	2.297478	2.921158
H	5.797605	0.706652	3.504085

CP'-1g-t

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.208037

Total energy: -4846.475454850

Ni	-0.911226	-1.008508	-0.061457
N	-2.681615	-0.721294	0.667994
C	-3.097416	0.497430	0.309442
C	-3.819620	-1.366045	1.293541
C	-4.742689	-0.191053	1.619527
H	-4.307966	-2.086562	0.605027
H	-5.813940	-0.402691	1.490914
N	-1.051530	0.843362	-0.797627
C	-0.348072	1.947642	-1.415874
C	-2.238218	1.322322	-0.425351
C	-1.469977	2.942442	-1.720907

H	0.408206	2.386193	-0.729374
H	-1.857744	2.815471	-2.749189
O	-4.356039	0.827805	0.692661
O	-2.504674	2.601734	-0.791918
H	-3.540341	-1.932935	2.197395
H	-4.579245	0.181532	2.648356
H	0.197102	1.643470	-2.326556
H	-1.196624	3.997927	-1.578484
Br	1.143507	-1.922624	-0.732873
C	2.421861	-0.665398	-0.047136
C	3.771982	-0.857240	-0.315012
C	1.965195	0.406610	0.709541
C	4.685431	0.064232	0.192039
H	4.110511	-1.712444	-0.906742
C	2.898938	1.312977	1.205765
H	0.890031	0.525453	0.889708
C	4.268264	1.162620	0.954486
H	5.752770	-0.076525	-0.008954
H	2.552321	2.160720	1.806708
C	5.258353	2.162197	1.465443
H	4.905858	2.645946	2.388740
H	6.235664	1.698050	1.666652
H	5.428509	2.963262	0.725627

CP'-1h-t

Geometry with 45 atoms:

Thermal correction to Gibbs Free Energy: 0.286555

Total energy: -5095.454269000

C	-2.535205	3.074631	-0.060110
C	-1.521185	2.171549	-0.344207
N	-1.747165	0.855505	-0.392485
C	-2.979553	0.307042	-0.168014
C	-4.053740	1.182287	0.138625
C	-3.828161	2.542016	0.191651
C	-0.109563	2.514919	-0.636227
C	-3.010246	-1.118003	-0.283811
C	-4.184322	-1.908572	-0.182397
C	-4.113965	-3.273585	-0.331408
C	-2.859914	-3.881103	-0.587632
C	-1.751213	-3.055738	-0.674322
N	0.697802	1.460125	-0.899032
N	-1.788361	-1.727174	-0.532803
C	1.968527	1.684832	-1.234772
C	2.521420	2.959833	-1.299068
C	1.709144	4.046712	-0.987059
C	0.376426	3.822096	-0.657975
Ni	-0.234430	-0.367603	-0.398155
H	-2.358259	4.151699	-0.029193
H	-5.053066	0.783990	0.337436
H	-4.652996	3.219349	0.429822
H	-5.145247	-1.421375	0.008018
H	-5.019926	-3.882164	-0.255708
H	-2.757796	-4.961286	-0.711896
H	-0.760770	-3.489416	-0.871457
H	2.577323	0.801829	-1.459838
H	3.568363	3.089856	-1.580768
H	2.106544	5.064677	-1.008619
H	-0.286528	4.657483	-0.422056
Br	3.824355	-1.829881	-0.399416
C	2.514478	-0.966972	0.673096
C	2.843128	0.187427	1.353306
C	1.214126	-1.519294	0.726258
C	1.856449	0.832689	2.127792
H	3.851979	0.603827	1.284225
C	0.247222	-0.873803	1.540883
H	1.047293	-2.536164	0.353236
C	0.575364	0.321653	2.242475
H	2.115081	1.760374	2.650516
H	-0.670010	-1.405008	1.826639
C	-0.486084	0.995455	3.048983
H	-1.336985	1.283718	2.403947
H	-0.895396	0.320060	3.819292
H	-0.112734	1.901666	3.548126

CP-1a'-s

Geometry with 37 atoms:

Thermal correction to Gibbs Free Energy: 0.221295

Total energy: -7422.571427760

Ni	0.488783	-0.278419	-0.559827
C	0.908935	-0.530902	1.473848
C	-1.547200	-1.762230	2.081033
C	0.660162	-1.850078	1.031538
C	-0.048267	0.152850	2.260200
C	-1.260634	-0.447845	2.524204
C	-0.574487	-2.446475	1.367752
H	1.463277	-2.453633	0.599932
H	0.173024	1.160708	2.627035
H	-2.017470	0.098491	3.098046
H	-0.764727	-3.477539	1.049368
N	-1.504542	-0.263225	-0.850347
C	-4.262595	-0.076843	-0.934264
C	-2.244149	-1.340231	-1.115323
C	-2.099873	0.925647	-0.649020
C	-3.490545	1.049984	-0.674629
C	-3.631710	-1.295677	-1.173366
N	0.135435	1.754082	-0.521845
C	-0.653357	4.354115	0.038026
C	1.042375	2.719579	-0.366804

C	-1.174963	2.056724	-0.426379
C	-1.602615	3.353975	-0.142236
C	0.696274	4.036340	-0.083412
H	-1.693034	-2.271378	-1.289821
H	-3.968586	2.016050	-0.502412
H	-4.201818	-2.199760	-1.395739
H	2.091738	2.419721	-0.467197
H	-2.666423	3.583971	-0.057824
H	1.473928	4.792689	0.039727
Br	1.709192	-1.354380	-2.342062
Br	2.719098	0.119046	1.462728
C	-2.875777	-2.375255	2.391884
H	-0.968079	5.375105	0.266904
H	-5.352277	0.000078	-0.958746
H	-3.696984	-1.757797	1.987678
H	-2.970258	-3.384039	1.962505
H	-3.044113	-2.448328	3.479421

CP-1b'-s

Geometry with 61 atoms:

Thermal correction to Gibbs Free Energy: 0.432757

Total energy: -7736.956193040

Ni	1.411466	-0.785978	-0.631995
C	-0.560877	1.291180	-0.390996
C	-1.149895	2.524356	-0.135702
C	-0.365746	3.681251	-0.033885
C	1.010627	3.522032	-0.214444
C	1.530145	2.255278	-0.462342
C	-1.326419	0.034564	-0.552004
C	-2.703154	-0.057978	-0.382390
C	-3.366121	-1.276040	-0.584906
C	-2.582662	-2.351697	-1.009352
C	-1.206987	-2.191415	-1.132518
H	-2.234824	2.589094	-0.022175
H	1.696509	4.369098	-0.165466
H	2.606649	2.106330	-0.607095
H	-3.265711	0.825929	-0.072740
H	-3.016512	-3.329759	-1.223436
H	-0.572619	-3.033258	-1.431064
N	0.772484	1.166016	-0.538259
N	-0.586757	-1.040767	-0.887570
C	-1.022682	5.023789	0.255829
C	-4.858174	-1.389994	-0.308934
C	-5.619586	-0.352717	-1.138884
H	-6.701337	-0.437073	-0.942347
H	-5.321594	0.680244	-0.898508
H	-5.456893	-0.512008	-2.218000
C	-5.082754	-1.131487	1.185598
H	-6.153554	-1.232337	1.429898
H	-4.522690	-1.858151	1.799285
H	-4.764718	-0.119561	1.484373
C	-5.395104	-2.776407	-0.648670
H	-5.257240	-3.021992	-1.714904
H	-4.913434	-3.564846	-0.046250
H	-6.475626	-2.815554	-0.436463
C	-2.036103	5.334188	-0.850494
H	-2.836221	4.578984	-0.909242
H	-2.514367	6.309115	-0.658202
H	-1.543288	5.385304	-1.835860
C	-1.739095	4.940958	1.607771
H	-1.028040	4.710002	2.418680
H	-2.217659	5.907188	1.839367
H	-2.526016	4.169728	1.616041
C	-0.002717	6.155869	0.313227
H	0.742964	5.999091	1.110320
H	0.532489	6.277329	-0.643224
H	-0.518249	7.106196	0.526053
Br	3.310046	-0.033634	1.683933
C	1.762126	-1.138322	1.379761
C	1.930135	-2.398564	0.751846
C	0.613578	-0.886154	2.172904
C	0.921646	-3.375267	0.932039
H	2.902182	-2.690317	0.343397
C	-0.365277	-1.848145	2.277922
H	0.511715	0.078091	2.681310
C	-0.227397	-3.118187	1.662016
H	1.062206	-4.363847	0.480404
H	-1.269719	-1.633986	2.859421
C	-1.305555	-4.142057	1.830959
H	-1.117385	-5.037887	1.220102
H	-1.398427	-4.461853	2.882747
H	-2.289207	-3.732175	1.539581
Br	3.145033	-0.997528	-2.308946

CP-1c'-s

Geometry with 45 atoms:

Thermal correction to Gibbs Free Energy: 0.281096

Total energy: -7651.598128220

Ni	0.484412	-0.916084	-0.632168
C	0.616377	-1.549319	1.323986
C	-2.112872	-2.227021	1.560489
C	0.099636	-2.654732	0.598876
C	-0.231314	-0.805143	2.185435
C	-1.566781	-1.125882	2.269583
C	-1.270094	-2.978069	0.758782
H	0.776457	-3.379439	0.136079
H	0.185884	0.024504	2.765251
H	-2.225158	-0.525200	2.907777

H	-1.666235	-3.855322	0.234654
N	-1.329438	0.002905	-0.793035
C	-3.734619	1.379530	-0.491291
C	-2.495130	-0.585395	-1.051138
C	-1.329469	1.301962	-0.423629
C	-2.505813	2.013488	-0.253826
C	-3.724228	0.049737	-0.927895
N	1.044613	1.054574	-0.436381
C	1.520820	3.725050	0.196741
C	2.285309	1.525092	-0.344591
C	0.012832	1.900673	-0.237923
C	0.211860	3.233872	0.083419
C	2.585621	2.845381	-0.033113
H	-2.451816	-1.631277	-1.373643
H	-2.513280	3.058642	0.061443
H	-4.637638	-0.499335	-1.160669
H	3.090095	0.804678	-0.532452
H	-0.617522	3.925331	0.245047
H	3.628190	3.160832	0.024059
Br	1.823441	-1.873700	-2.417356
Br	2.512815	-1.455052	1.649973
C	-3.564493	-2.557709	1.711413
O	1.650089	5.012154	0.510532
O	-4.831004	2.105523	-0.289939
C	2.944656	5.563758	0.632725
H	2.815200	6.620829	0.892566
H	3.519240	5.064811	1.430928
H	3.502126	5.492314	-0.316130
C	-6.095252	1.506993	-0.488309
H	-6.232883	0.636574	0.175438
H	-6.847305	2.266356	-0.244822
H	-6.229312	1.190885	-1.536198
H	-3.866749	-3.380624	1.046281
H	-3.806146	-2.852642	2.746709
H	-4.196833	-1.682601	1.479566

CP-1d'-s

Geometry with 43 atoms:

Thermal correction to Gibbs Free Energy: 0.272293

Total energy: -7501.201156790

Ni	0.085617	0.964152	-0.694938
C	-1.823338	-0.937509	1.358917
C	0.807453	-1.482197	2.146704
C	-1.034768	0.090985	1.870677
C	-1.311885	-2.223938	1.204159
C	0.000237	-2.483415	1.592160
C	0.270280	-0.196852	2.267016
H	-1.442341	1.099870	1.978653
H	-1.934605	-3.018953	0.782911
H	0.405381	-3.493831	1.466649
H	0.889214	0.604075	2.687804
N	1.998042	0.982012	-0.123069
C	4.658684	0.706059	0.596664
C	2.623752	1.989298	0.508112
C	2.659534	-0.160591	-0.395727
C	4.000697	-0.330068	-0.056060
C	3.963420	1.874578	0.887636
N	0.600814	-0.810153	-1.395368
C	1.487736	-3.356122	-2.035548
C	-0.215107	-1.654157	-2.048911
C	1.852515	-1.194750	-1.072533
C	2.331212	-2.467450	-1.378000
C	0.205905	-2.944608	-2.380788
H	4.525275	-1.257698	-0.292718
H	4.449020	2.706184	1.404095
H	3.345542	-2.764469	-1.104746
H	-0.477210	-3.611843	-2.912262
Br	-1.575219	2.594917	-0.893475
Br	-3.629603	-0.588290	0.889643
C	2.196450	-1.784736	2.616038
H	5.708982	0.600416	0.878925
H	1.833510	-4.362519	-2.283831
C	1.825279	3.218538	0.770438
H	1.549038	3.704789	-0.180228
H	0.874138	2.962595	1.265417
H	2.376697	3.939811	1.388687
C	-1.571447	-1.149083	-2.398071
H	-2.221748	-1.126689	-1.506057
H	-1.505836	-0.110826	-2.760755
H	-2.057067	-1.777441	-3.157426
H	2.832299	-0.885031	2.606547
H	2.192484	-2.168467	3.650965
H	2.677048	-2.555107	1.991498

CP-1e'-s

Geometry with 39 atoms:

Thermal correction to Gibbs Free Energy: 0.235222

Total energy: -7498.772735380

Ni	0.708984	0.110694	0.652921
C	1.244581	0.831616	-1.216840
C	-0.219620	3.231708	-0.972845
C	1.660348	1.819890	-0.288812
C	0.104346	1.057038	-2.029898
C	-0.618633	2.219541	-1.882367
C	0.915455	3.020359	-0.207613
H	2.651836	1.765715	0.170547
H	-0.192150	0.299697	-2.762613
H	-1.517255	2.374526	-2.490538

H	1.257765	3.804973	0.476595
N	-1.240216	0.692234	0.928322
C	-3.976393	1.250589	0.840652
C	-1.713065	1.843124	1.378332
C	-2.114629	-0.224977	0.452675
C	-3.504571	0.003981	0.378886
C	-3.080923	2.164372	1.355246
N	-0.241274	-1.654605	0.131726
C	-1.853479	-3.718831	-0.828649
C	0.284514	-2.818921	-0.207686
C	-1.577813	-1.486781	0.025637
C	-2.441824	-2.491170	-0.458833
C	-0.490458	-3.885480	-0.694546
H	-3.413361	3.131327	1.738555
H	-0.006276	-4.826815	-0.961955
Br	2.396890	-0.510012	2.278033
Br	2.520123	-0.477314	-1.819900
C	-1.010795	4.498274	-0.877474
H	-5.046881	1.471734	0.797238
H	-2.486334	-4.525800	-1.209640
H	1.370212	-2.916989	-0.090609
H	-0.981989	2.556301	1.773941
C	-3.847892	-2.223996	-0.539576
C	-4.357189	-1.025666	-0.139533
H	-4.504341	-3.009999	-0.923994
H	-5.431625	-0.828554	-0.196761
H	-0.959783	5.076212	-1.815899
H	-2.079277	4.288640	-0.698358
H	-0.648843	5.144562	-0.063812

CP-1f'-s

Geometry with 43 atoms:

Thermal correction to Gibbs Free Energy: 0.271233

Total energy: -7501.175181550

Ni	0.777722	-0.369754	-0.564675
C	1.280135	-0.488630	1.455879
C	-0.901273	-2.118927	2.166939
C	1.255419	-1.841517	1.045479
C	0.239824	0.034344	2.260586
C	-0.838955	-0.763466	2.574887
C	0.155437	-2.637857	1.434457
H	2.141724	-2.307021	0.605472
H	0.289910	1.074251	2.600214
H	-1.664274	-0.344692	3.161673
H	0.141382	-3.693898	1.142239
N	-1.201070	-0.679531	-0.774272
C	-3.977527	-0.953386	-0.663991
C	-1.774692	-1.867420	-0.970696
C	-1.974795	0.397728	-0.559325
C	-3.363682	0.288929	-0.490007
C	-3.148230	-2.049334	-0.933605
N	0.098454	1.581218	-0.564532
C	-1.103881	4.063976	-0.073640
C	0.831278	2.692508	-0.482002
C	-1.238895	1.674270	-0.424175
C	-1.862402	2.894894	-0.174763
C	0.279888	3.942756	-0.237756
H	-1.093319	-2.703525	-1.165758
H	-3.981420	1.171090	-0.303512
H	-3.573916	-3.042212	-1.102768
H	1.913069	2.570235	-0.608319
H	-2.947486	2.947502	-0.052725
H	0.927810	4.821050	-0.171842
Br	2.104086	-1.270852	-2.374685
Br	2.950954	0.464446	1.388387
C	-1.747041	5.388067	0.169905
C	-5.455901	-1.116150	-0.548275
H	-1.947533	5.897829	-0.787724
H	-1.093960	6.050837	0.756389
H	-2.709359	5.282602	0.691265
H	-5.842475	-1.815373	-1.304882
H	-5.983147	-0.156816	-0.647285
H	-5.714798	-1.538405	0.437744
C	-2.088865	-2.949793	2.538589
H	-2.028007	-3.962198	2.111879
H	-2.189935	-3.045864	3.632871
H	-3.023632	-2.485790	2.177109

CP-1g'-s

Geometry with 35 atoms:

Thermal correction to Gibbs Free Energy: 0.209263

Total energy: -7420.622404570

C	1.022758	1.000657	-1.143300
C	-1.211366	2.709391	-1.151304
C	0.890458	1.979460	-0.129072
C	0.062701	0.901425	-2.177468
C	-1.040598	1.726479	-2.157970
C	-0.239832	2.831047	-0.171751
H	1.728461	2.217336	0.532692
H	0.199017	0.162383	-2.973185
H	-1.797932	1.630354	-2.943658
H	-0.337963	3.610469	0.592205
Br	1.517530	-0.108913	2.707688
Br	2.723049	0.134914	-1.381319
C	-2.416746	3.596248	-1.180122
H	-2.431903	4.293077	-0.328720
H	-2.456234	4.192091	-2.107456
H	-3.348278	3.004691	-1.153030

Ni	0.410661	-0.009206	0.571595
N	-0.128860	-1.836115	-0.385668
C	-1.401294	-1.966393	-0.412121
C	0.409381	-2.931059	-1.186550
C	-0.829698	-3.754298	-1.576914
H	0.946825	-2.516660	-2.056943
H	-0.967938	-3.869891	-2.660662
N	-1.621457	0.034984	0.807741
C	-2.649685	0.811830	1.489819
C	-2.216735	-0.962644	0.271063
C	-3.959183	0.156315	1.029169
H	-2.487304	0.746695	2.579353
H	-4.505987	0.756987	0.285225
O	-1.943288	-2.981833	-1.063072
O	-3.529680	-1.064364	0.373304
H	1.143920	-3.506995	-0.602448
H	-0.864287	-4.747774	-1.106143
H	-2.580086	1.875916	1.214835
H	-4.644084	-0.114205	1.843121

CP-1h'-s

Geometry with 46 atoms:

Thermal correction to Gibbs Free Energy: 0.283888

Total energy: -7669.602693620

C	2.712865	1.163650	-2.042727
C	1.421417	1.151247	-1.517868
N	0.772401	-0.006590	-1.315484
C	1.370913	-1.188879	-1.532040
C	2.660690	-1.250600	-2.057706
C	3.325743	-0.055565	-2.332389
C	0.646722	2.328913	-1.086380
C	0.546437	-2.336970	-1.113318
C	0.991002	-3.660257	-1.123016
C	0.153080	-4.654420	-0.630858
C	-1.109193	-4.305023	-0.152233
C	-1.484350	-2.966507	-0.192468
N	-0.592822	2.048673	-0.629197
N	-0.680180	-2.008359	-0.653277
C	-1.355040	3.036087	-0.158787
C	-0.922240	4.356506	-0.104408
C	0.353927	4.656182	-0.579976
C	1.147773	3.631921	-1.083264
Ni	-1.063715	0.029443	-0.684830
H	3.239428	2.104157	-2.220796
H	3.146212	-2.210619	-2.247662
H	4.333535	-0.074740	-2.754402
H	1.986638	-3.908493	-1.498323
H	0.484288	-5.695842	-0.619249
H	-1.795068	-5.056444	0.244567
H	-2.470145	-2.632088	0.154350
H	-2.355634	2.742272	0.182556
H	-1.575242	5.132624	0.300247
H	0.729628	5.682205	-0.557879
H	2.152900	3.840517	-1.457311
Br	-3.487103	0.087752	-0.778440
C	0.675267	-0.038574	2.106497
C	1.332408	-1.256056	1.945855
C	1.358021	1.167092	1.964462
C	2.686205	-1.256695	1.620440
H	0.788640	-2.198631	2.064759
C	2.711706	1.143952	1.639252
H	0.834340	2.119124	2.097593
C	3.399455	-0.062453	1.458505
H	3.201634	-2.214552	1.483349
H	3.247471	2.092673	1.517416
C	4.843676	-0.074814	1.067680
H	5.359033	-0.972219	1.442417
H	4.951017	-0.075986	-0.031850
H	5.374237	0.813682	1.442315
Br	-1.174143	-0.022624	2.528363

TS1a,3a

Geometry with 36 atoms:

Thermal correction to Gibbs Free Energy: 0.221374

Total energy: -4848.419973520

C	2.463233	0.663708	-0.661646
C	1.814366	-0.393741	-0.014894
C	1.874912	-0.543768	1.376605
C	2.504033	0.443671	2.120983
C	3.110209	1.556634	1.510839
C	3.076502	1.646743	0.116085
Br	1.540754	-2.146426	-1.200098
H	1.401029	-1.400566	1.866164
H	2.470003	0.735820	-1.754921
H	3.553826	2.498499	-0.381007
H	2.526733	0.355107	3.213247
C	-2.479646	-0.140489	0.488062
C	-1.615675	-2.298106	0.831589
C	-2.694841	-2.680168	1.602575
C	-3.722691	-1.729828	1.823312
C	-3.613011	-0.475413	1.270866
C	-2.262422	1.130071	-0.132890
C	-0.797600	2.412856	-1.456330
C	-1.624297	3.515710	-1.419344
C	-2.841202	3.410931	-0.697498
C	-3.151059	2.231966	-0.061747
H	-0.796644	-3.001751	0.632453
H	-2.743652	-3.687336	2.022770

H	-4.396859	0.269448	1.434347
H	0.155956	2.445234	-1.999194
H	-1.339423	4.436468	-1.933489
H	-4.083429	2.138152	0.501797
N	-1.489315	-1.080673	0.283042
N	-1.086654	1.249950	-0.848855
Ni	0.019295	-0.349295	-0.764154
C	3.793393	2.592810	2.344353
H	-3.527578	4.261100	-0.643330
H	-4.596712	-1.989200	2.428044
H	4.099641	3.462035	1.743280
H	3.138875	2.950361	3.156617
H	4.698130	2.185354	2.828145

TS1b,3b

Geometry with 60 atoms:

Thermal correction to Gibbs Free Energy: 0.428372

Total energy: -5162.800649720

C	3.622515	1.074765	-0.057244
C	3.102699	-0.211438	0.127271
C	2.969959	-0.766835	1.407078
C	3.260899	0.028291	2.505828
C	3.720771	1.350078	2.361564
C	3.894696	1.852968	1.068983
Br	3.357074	-1.531175	-1.520558
H	2.604728	-1.790930	1.534558
H	3.788879	1.475476	-1.063417
H	4.265771	2.874941	0.933541
H	3.125893	-0.382757	3.512952
C	-1.196782	-0.710868	-0.232373
C	-0.013243	-2.723555	-0.333419
C	-1.112727	-3.466392	0.050571
C	-2.341279	-2.799579	0.312651
C	-2.353212	-1.424611	0.161988
C	-1.129401	0.708565	-0.404729
C	0.242524	2.525599	-0.956252
C	-0.779537	3.430235	-0.782184
C	-2.073515	2.959594	-0.396214
C	-2.216560	1.600052	-0.213439
H	0.942122	-3.223834	-0.540640
H	-1.010131	-4.548906	0.142906
H	-3.272748	-0.863365	0.354092
H	1.243579	2.868139	-1.249476
H	-0.583600	4.493996	-0.941496
H	-3.180189	1.181484	0.085944
N	-0.023080	-1.394109	-0.479210
N	0.102391	1.200698	-0.786936
Ni	1.467369	-0.175715	-0.923355
C	4.032255	2.173847	3.569660
C	-3.209386	3.955243	-0.206578
C	-3.603905	-3.538034	0.751157
C	-4.728153	-3.267051	-0.251804
H	-5.645278	-3.805202	0.045533
H	-4.978684	-2.195395	-0.315044
H	-4.449167	-3.609300	-1.263587
C	-3.385194	-5.045315	0.830957
H	-2.607078	-5.312941	1.565775
H	-4.319077	-5.540588	1.145984
H	-3.097189	-5.473880	-0.144061
C	-4.024408	-3.037748	2.135817
H	-4.930012	-3.569096	2.477671
H	-3.228420	-3.213874	2.880189
H	-4.252003	-1.958980	2.134335
C	-4.509174	3.275886	0.207791
H	-5.302410	4.032048	0.332416
H	-4.857952	2.553756	-0.549908
H	-4.408497	2.741963	1.168037
C	-3.449091	4.698397	-1.524198
H	-3.732748	3.997437	-2.328559
H	-4.268082	5.429679	-1.408687
H	-2.555859	5.251582	-1.858303
C	-2.820268	4.960788	0.881243
H	-2.638317	4.452327	1.844128
H	-1.910159	5.525734	0.620594
H	-3.632187	5.693129	1.033929
H	3.170355	2.219625	4.256490
H	4.868174	1.741363	4.146131
H	4.308295	3.204113	3.299685

TS1c,3c

Geometry with 44 atoms:

Thermal correction to Gibbs Free Energy: 0.278461

Total energy: -5077.438233340

C	3.077912	0.915539	-0.195147
C	2.482616	-0.328816	0.038532
C	2.425597	-0.878275	1.325945
C	2.875609	-0.112599	2.391883
C	3.418686	1.171162	2.203431
C	3.509970	1.666050	0.899275
Br	2.506487	-1.666759	-1.627319
H	1.998790	-1.872777	1.489824
H	3.182214	1.307472	-1.213027
H	3.943214	2.657631	0.727636
H	2.803386	-0.517637	3.407846
C	-1.864332	-0.524201	0.007251
C	-0.810967	-2.612448	-0.094422
C	-1.920754	-3.288490	0.383577
C	-3.073424	-2.516350	0.689869

C	-3.038633	-1.146814	0.501157
C	-1.724111	0.875091	-0.226982
C	-0.276970	2.578478	-0.939625
C	-1.221647	3.571504	-0.754094
C	-2.500908	3.175578	-0.274504
C	-2.741535	1.839616	-0.013163
H	0.097553	-3.177335	-0.343047
H	-1.883858	-4.371206	0.510368
H	-3.929688	-0.561441	0.743450
H	0.723950	2.844645	-1.304054
H	-0.967901	4.609687	-0.971866
H	-3.727621	1.547537	0.358140
N	-0.751463	-1.295109	-0.285333
N	-0.487868	1.281966	-0.703618
Ni	0.776282	-0.189808	-0.884528
C	3.900015	1.963423	3.376344
O	-3.507116	4.037634	-0.053754
O	-4.215139	-3.044472	1.160938
C	-3.307501	5.405189	-0.317867
H	-4.247737	5.918498	-0.074945
H	-2.503566	5.833883	0.306094
H	-3.072369	5.590300	-1.380853
C	-4.293509	-4.435112	1.360612
H	-5.301480	-4.647407	1.741892
H	-4.149818	-4.995878	0.420161
H	-3.556648	-4.788054	2.103548
H	3.103076	2.089176	4.128639
H	4.735393	1.455753	3.888479
H	4.246822	2.963887	3.077420

TS1d,3d

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.27275

Total energy: -4927.025493040

C	-1.395716	-0.503376	1.654326
C	-1.745388	0.026038	0.404210
C	-2.143398	1.361474	0.279997
C	-2.017561	2.205269	1.379923
C	-1.570549	1.730559	2.619159
C	-1.280983	0.361666	2.735137
Br	-2.501943	-1.272015	-1.067620
H	-2.510179	1.748534	-0.675171
H	-1.169573	-1.567469	1.772197
H	-0.961815	-0.039405	3.703727
H	-2.286528	3.262004	1.272376
C	2.282244	-0.525826	0.230360
C	1.335588	-2.692359	0.308063
C	2.400096	-3.170387	1.057917
C	3.436739	-2.279002	1.423091
C	3.380552	-0.970635	1.008539
C	2.161152	0.794986	-0.304876
C	0.879518	2.198542	-1.719809
C	1.796650	3.232383	-1.587884
C	2.921843	3.042295	-0.751972
C	3.105804	1.835789	-0.118890
H	2.425135	-4.222929	1.352466
H	4.181176	-0.272805	1.267389
H	1.635725	4.171480	-2.124596
H	3.977399	1.673884	0.520795
N	1.261115	-1.403541	-0.085786
N	1.046911	1.020082	-1.090420
Ni	-0.267889	-0.411096	-0.882256
C	-1.410080	2.643475	3.791671
H	3.648578	3.849064	-0.616308
H	4.281766	-2.631521	2.022164
C	-0.347105	2.356204	-2.558023
H	-0.763560	1.375368	-2.844104
H	-1.129641	2.914820	-2.016051
H	-0.131886	2.921937	-3.477682
C	0.217900	-3.590218	-0.104950
H	-0.735122	-3.288336	0.362412
H	0.063322	-3.545220	-1.196576
H	0.415292	-4.634526	0.176329
H	-0.344003	2.854718	3.987757
H	-1.911239	3.609286	3.627077
H	-1.815983	2.195269	4.713161

TS1e,3e

Geometry with 38 atoms:

Thermal correction to Gibbs Free Energy: 0.233191

Total energy: -4924.619437000

C	2.687298	0.918065	-0.589064
C	2.148928	-0.195265	0.065835
C	2.147351	-0.287546	1.463886
C	2.594460	0.800846	2.198521
C	3.081278	1.964533	1.575417
C	3.117283	2.001586	0.178517
Br	2.184277	-2.009929	-1.055459
H	1.763262	-1.183382	1.962406
H	2.747283	0.953308	-1.682726
H	3.504926	2.892791	-0.327424
H	2.565006	0.754334	3.293274
C	-2.144344	-0.507309	0.262085
C	-1.098693	-2.523313	0.775630
C	-2.209652	-2.974506	1.478789
C	-3.342613	-2.147457	1.572436
C	-3.324449	-0.894702	0.961859
C	-2.060180	0.744787	-0.372306

C	-0.776708	2.239489	-1.625460
C	-1.794250	3.179576	-1.629454
C	-3.008343	2.886327	-0.973917
C	-3.152814	1.657516	-0.331385
H	-2.188685	-3.962176	1.945492
H	-1.643202	4.135065	-2.137757
N	-1.042073	-1.331345	0.174238
N	-0.881413	1.041348	-1.027518
Ni	0.419408	-0.398809	-0.799854
C	3.565107	3.113308	2.400857
H	-3.832263	3.607052	-0.959086
H	-4.235418	-2.471511	2.117146
C	-4.337150	1.249620	0.378312
C	-4.419086	0.037369	0.992981
H	-5.328558	-0.253987	1.529360
H	-5.180335	1.947958	0.413005
H	0.176966	2.448752	-2.126098
H	-0.205038	-3.154762	0.688259
H	2.796888	3.440973	3.121329
H	4.452449	2.835089	2.995348
H	3.837471	3.977107	1.776176

TS1f,3f

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.270522

Total energy: -4927.022383940

C	2.810690	0.865319	-0.415752
C	2.198889	-0.302084	0.053623
C	2.146415	-0.597840	1.422180
C	2.616251	0.348494	2.321241
C	3.175345	1.565035	1.889586
C	3.263267	1.802054	0.514716
Br	2.183486	-1.929508	-1.328456
H	1.706149	-1.536911	1.772494
H	2.909816	1.056479	-1.490029
H	3.709342	2.736326	0.156073
H	2.547313	0.144127	3.395958
C	-2.138678	-0.463564	0.151366
C	-1.139365	-2.578193	0.301094
C	-2.255120	-3.135609	0.887714
C	-3.392390	-2.310875	1.124241
C	-3.313484	-0.985820	0.751099
C	-1.970017	0.894352	-0.265397
C	-0.504434	2.453855	-1.232353
C	-1.422389	3.475313	-1.130889
C	-2.702023	3.197863	-0.565568
C	-2.951956	1.910575	-0.140319
H	-0.249534	-3.191575	0.106389
H	-2.264030	-4.193932	1.165131
H	-4.170581	-0.326471	0.922245
H	0.489738	2.637025	-1.660822
H	-1.170945	4.481913	-1.478090
H	-3.923687	1.669694	0.303090
N	-1.056162	-1.291379	-0.066033
N	-0.745498	1.196279	-0.828438
Ni	0.475925	-0.318094	-0.843857
C	-3.715208	4.286343	-0.447742
H	-4.652034	3.930503	0.006866
H	-3.331217	5.121490	0.163971
H	-3.953913	4.715294	-1.436741
C	-4.613848	-2.888816	1.756405
H	-5.409189	-2.138363	1.879661
H	-5.016597	-3.721133	1.153081
H	-4.383816	-3.313020	2.749412
C	3.675220	2.558800	2.888478
H	2.879530	2.851235	3.594488
H	4.494277	2.139502	3.497628
H	4.050108	3.471706	2.402107

TS1g,3g

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.207965

Total energy: -4846.470727620

C	2.328643	0.400201	-0.832655
C	1.654644	-0.473025	0.031226
C	1.702335	-0.298400	1.422235
C	2.338828	0.825023	1.927160
C	2.968465	1.761198	1.085349
C	2.951097	1.527476	-0.292277
Br	1.315143	-2.420909	-0.714537
H	1.202338	-1.011162	2.085903
H	2.342372	0.221535	-1.913492
H	3.446985	2.235744	-0.965506
H	2.347919	0.991983	3.010554
Ni	-0.115083	-0.470753	-0.742837
C	3.652696	2.956052	1.668711
H	4.009522	3.643275	0.886913
H	2.978567	3.518629	2.336389
H	4.523930	2.662937	2.279920
N	-1.661785	-0.980718	0.389243
C	-2.508902	0.042314	0.460320
C	-2.210196	-2.034446	1.216496
C	-3.276922	-1.305998	2.037122
H	-2.646260	-2.846808	0.599846
H	-4.207720	-1.873956	2.179886
N	-1.128406	1.172589	-1.065757
C	-1.089743	2.444937	-1.758247
C	-2.225041	1.183495	-0.305192

C	-2.112928	3.283883	-0.991051
H	-0.083555	2.898756	-1.736240
H	-2.739926	3.927468	-1.624992
O	-3.568193	-0.121357	1.279816
O	-2.950839	2.319569	-0.336425
H	-1.443610	-2.503199	1.858393
H	-2.894466	-1.004285	3.029819
H	-1.367029	2.333893	-2.826070
H	-1.631032	3.913022	-0.219815

TS1h,3h

Geometry with 45 atoms:

Thermal correction to Gibbs Free Energy: 0.286362

Total energy: -5095.445774350

C	1.156027	3.201133	-0.799744
C	1.164964	1.803335	-0.965551
N	-0.027921	1.146002	-1.054784
C	-1.209098	1.779916	-0.960112
C	-1.275127	3.153306	-0.796873
C	-0.055350	3.869577	-0.718413
C	2.308753	0.932424	-1.037037
C	-2.356881	0.855986	-1.034813
C	-3.690367	1.273022	-1.057668
C	-4.699740	0.322788	-1.131685
C	-4.355994	-1.029818	-1.186591
C	-3.009755	-1.367855	-1.155147
N	2.018995	-0.414865	-1.111190
N	-2.032898	-0.460275	-1.077375
C	3.031205	-1.287400	-1.180814
C	4.366338	-0.922746	-1.176613
C	4.676827	0.453780	-1.096986
C	3.651604	1.371586	-1.030322
Ni	0.020955	-0.760823	-0.722827
H	2.094999	3.757097	-0.723099
H	-2.231811	3.675234	-0.719800
H	-0.071275	4.954061	-0.582653
H	-3.931035	2.338087	-1.021020
H	-5.747729	0.632595	-1.149315
H	-5.117111	-1.810310	-1.249234
H	-2.694406	-2.418034	-1.179403
H	2.746335	-2.346930	-1.227589
H	5.147150	-1.684258	-1.233492
H	5.717768	0.789152	-1.089641
H	3.868886	2.441997	-0.971908
C	0.026815	-1.000252	1.318736
C	1.226189	-0.479630	1.836677
C	-1.198321	-0.567042	1.858337
C	1.179619	0.614323	2.691993
H	2.189908	-0.887541	1.518591
C	-1.217676	0.528907	2.710923
H	-2.134567	-1.048634	1.561665
C	-0.036338	1.165495	3.120429
H	2.121626	1.055629	3.037447
H	-2.182816	0.900873	3.073771
Br	0.072672	-2.898819	0.546166
C	-0.075494	2.386913	3.983749
H	-0.937669	2.374682	4.668912
H	0.841332	2.491363	4.584314
H	-0.166253	3.304144	3.374398

TS'1a,3a

Geometry with 36 atoms:

Thermal correction to Gibbs Free Energy: 0.217108

Total energy: -4848.408086730

Ni	-0.726607	-0.944600	-0.438174
C	2.694283	-0.606516	-0.047603
C	4.055991	-0.818138	-0.136469
C	2.129434	0.388197	0.722287
C	4.894321	0.022332	0.602723
H	4.477599	-1.612670	-0.764431
C	2.982236	1.218542	1.453444
H	1.034913	0.516924	0.748072
C	4.372683	1.045878	1.406551
H	5.981472	-0.117130	0.553777
H	2.563012	2.021265	2.072689
Br	1.223675	-1.836295	-1.229410
N	-2.341224	-0.856439	0.592008
C	-4.778632	-0.492913	1.894374
C	-2.893007	-1.850178	1.309410
C	-2.993055	0.342770	0.509971
C	-4.222253	0.537802	1.158633
C	-4.097003	-1.719511	1.975471
N	-1.169154	0.915957	-0.889487
C	-2.003444	3.549173	-1.216172
C	-0.456656	1.770279	-1.637274
C	-2.310742	1.350994	-0.284077
C	-2.744455	2.677757	-0.438300
C	-0.828568	3.087830	-1.834767
H	-2.328790	-2.789027	1.342033
H	-4.736285	1.498839	1.075330
H	-4.498631	-2.558631	2.548209
H	0.452978	1.364453	-2.097533
H	-3.655940	3.018190	0.059708
H	-0.216378	3.743280	-2.458441
C	5.281724	1.918997	2.215275
H	-2.328679	4.585314	-1.343454
H	-5.736277	-0.352853	2.402944
H	6.244635	2.085147	1.706918

H	4.825938	2.900031	2.421048
H	5.512322	1.459601	3.192827

TS'1b,3b

Geometry with 60 atoms:

Thermal correction to Gibbs Free Energy: 0.426076

Total energy: -5162.790679010

Ni	0.639814	-1.297743	-0.989449
C	3.917642	-1.018052	0.093377
C	5.287622	-1.161696	0.188056
C	3.160672	-0.337167	1.023996
C	5.927964	-0.585755	1.290258
H	5.864246	-1.710786	-0.566572
C	3.816533	0.231176	2.117842
H	2.068966	-0.253852	0.896233
C	5.206566	0.118180	2.264390
H	7.014916	-0.686907	1.399524
H	3.240510	0.773790	2.877776
Br	2.763683	-1.824747	-1.650822
N	-1.133881	-1.595311	-0.323590
C	-3.821318	-1.729194	0.533007
C	-1.732515	-2.776466	-0.093070
C	-1.860280	-0.455860	-0.130896
C	-3.198221	-0.512303	0.294105
C	-3.040187	-2.892640	0.328400
N	0.124087	0.594716	-0.878136
C	-0.889505	3.191720	-0.465789
C	0.868973	1.677101	-1.144019
C	-1.137116	0.776141	-0.399821
C	-1.654254	2.066585	-0.190308
C	0.418129	2.968312	-0.961892
H	-1.116931	-3.667897	-0.258933
H	-3.741357	0.425378	0.428374
H	-3.453864	-3.890650	0.498119
H	1.879439	1.485047	-1.526371
H	-2.668933	2.167311	0.200262
H	1.082489	3.801854	-1.206020
C	5.906843	0.758595	3.422860
C	-5.268033	-1.852287	0.989637
C	-5.938721	-0.492678	1.145147
H	-5.964547	0.067035	0.194776
H	-6.981771	-0.628727	1.476088
H	-5.432938	0.134413	1.898846
C	-6.051013	-2.666139	-0.044685
H	-5.644057	-3.683102	-0.168991
H	-7.104663	-2.766295	0.268487
H	-6.036879	-2.172220	-1.031724
C	-5.305090	-2.571550	2.341070
H	-4.877226	-3.585928	2.284054
H	-4.742836	-2.008602	3.106146
H	-6.347173	-2.670183	2.691250
C	-1.390498	4.613427	-0.254066
C	-1.358996	5.358537	-1.591543
H	-2.008020	4.865682	-2.336009
H	-1.720882	6.392845	-1.459241
H	-0.341870	5.414659	-2.012941
C	-2.815273	4.646121	0.285794
H	-2.898600	4.144307	1.264736
H	-3.136477	5.692037	0.423223
H	-3.530648	4.169636	-0.405781
C	-0.473352	5.320837	0.747681
H	-0.472302	4.800245	1.721030
H	0.568461	5.374738	0.391378
H	-0.820456	6.354805	0.917125
H	5.266255	0.789011	4.318300
H	6.836347	0.227412	3.680810
H	6.186249	1.802405	3.194275

TS'1c,3c

Geometry with 44 atoms:

Thermal correction to Gibbs Free Energy: 0.275241

Total energy: -5077.429526940

Ni	-0.035502	-1.008615	-0.885274
C	3.319850	-0.921287	-0.038448
C	4.678538	-1.170736	-0.034805
C	2.680708	-0.200142	0.948774
C	5.431479	-0.664153	1.028798
H	5.160720	-1.749672	-0.832136
C	3.448282	0.298088	2.003489
H	1.592740	-0.032127	0.893978
C	4.831585	0.076421	2.057040
H	6.512122	-0.850130	1.064493
H	2.966153	0.870042	2.805953
Br	2.019338	-1.618205	-1.685712
N	-1.783866	-1.237846	-0.122988
C	-4.397929	-1.274140	0.881274
C	-2.410469	-2.390706	0.142921
C	-2.453882	-0.063181	0.110226
C	-3.762797	-0.067414	0.609562
C	-3.696941	-2.477694	0.642215
N	-0.463723	0.906902	-0.736418
C	-1.350850	3.523522	-0.312296
C	0.303532	1.954685	-1.046647
C	-1.700860	1.136292	-0.198878
C	-2.160241	2.442442	0.020405
C	-0.074779	3.273708	-0.866495
H	-1.840798	-3.305399	-0.057870
H	-4.304196	0.864984	0.789916

H	-4.133386	-3.458475	0.837223
H	1.288169	1.722260	-1.472400
H	-3.144089	2.636305	0.455675
H	0.608107	4.075034	-1.152617
C	5.655316	0.639515	3.173633
O	-1.840153	4.747122	-0.078497
O	-5.648200	-1.215516	1.355415
C	-1.050020	5.870556	-0.395492
H	-1.635431	6.758962	-0.124336
H	-0.105932	5.881580	0.176722
H	-0.817963	5.916407	-1.473758
C	-6.329968	-2.418054	1.630587
H	-7.326359	-2.142468	2.000264
H	-6.448466	-3.037465	0.724460
H	-5.816814	-3.011199	2.407417
H	6.062078	1.631844	2.909674
H	5.060564	0.770599	4.091060
H	6.516614	-0.005280	3.409196

TS'1d,3d

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.268679

Total energy: -4927.021284180

Ni	-0.589598	-0.007190	-0.949030
C	2.776157	-0.011758	-0.300421
C	4.150547	-0.010603	-0.433541
C	2.131359	-0.011718	0.919057
C	4.917249	-0.007334	0.735654
H	4.632436	-0.016456	-1.418572
C	2.913983	-0.008986	2.075636
H	1.028127	-0.017813	0.965166
C	4.313731	-0.003097	2.000776
H	6.011834	-0.011257	0.665833
H	2.430866	-0.014437	3.060434
Br	1.435270	-0.014410	-2.083872
N	-1.748895	-1.288724	-0.053826
C	-3.558323	-2.881372	1.327728
C	-1.626492	-2.632732	-0.090568
C	-2.747832	-0.716213	0.675823
C	-3.673488	-1.502876	1.374857
C	-2.514918	-3.457195	0.587485
N	-1.736530	1.294845	-0.066255
C	-3.532838	2.917850	1.297097
C	-1.601808	2.637214	-0.116297
C	-2.741233	0.738928	0.668264
C	-3.660560	1.540994	1.358037
C	-2.483332	3.476574	0.552474
H	-4.472543	-1.032704	1.952641
H	-2.390291	-4.541892	0.536751
H	-4.464646	1.083819	1.939216
H	-2.348622	4.559509	0.491013
C	5.146701	0.031463	3.246271
H	5.352779	1.069313	3.560754
H	4.638081	-0.463204	4.087938
H	6.121508	-0.457483	3.096553
C	-0.484895	-3.161130	-0.888751
H	-0.561302	-2.822372	-1.936441
H	0.465570	-2.753621	-0.501899
H	-0.438243	-4.258582	-0.870508
C	-0.454803	3.147438	-0.918489
H	0.491586	2.734850	-0.527123
H	-0.533544	2.799602	-1.962985
H	-0.398202	4.244551	-0.910451
H	-4.269447	-3.513164	1.866040
H	-4.238889	3.561491	1.828000

TS'1e,3e

Geometry with 38 atoms:

Thermal correction to Gibbs Free Energy: 0.231259

Total energy: -4924.607816020

Ni	-0.306996	-1.247896	-0.406417
C	3.001546	-0.415693	0.048103
C	4.380153	-0.398594	-0.033797
C	2.272846	0.510657	0.763941
C	5.060601	0.609818	0.655560
H	4.932973	-1.143602	-0.619280
C	2.969599	1.510392	1.446985
H	1.171939	0.456321	0.785761
C	4.369297	1.572826	1.404473
H	6.155943	0.653725	0.609997
H	2.417468	2.263009	2.023455
Br	1.775043	-1.922830	-1.078500
N	-1.955452	-1.243899	0.592344
C	-4.442741	-0.832604	1.842781
C	-2.482930	-2.165629	1.405881
C	-2.670620	-0.093519	0.384636
C	-3.921726	0.157983	0.997661
C	-3.711770	-2.003352	2.042926
N	-0.891362	0.536351	-1.044907
C	-2.101174	3.010993	-1.583408
C	-0.307187	1.425538	-1.847256
C	-2.090588	0.868727	-0.481797
C	-2.741835	2.101464	-0.729352
C	-0.871240	2.667799	-2.142353
H	-4.083864	-2.795664	2.696888
H	-0.344983	3.351817	-2.812344
C	5.114053	2.629939	2.159740
H	-2.572671	3.974714	-1.799843

H	-5.407736	-0.674602	2.334161
C	-4.573294	1.409276	0.724520
C	-4.008584	2.339301	-0.095822
H	-4.513164	3.291129	-0.290846
H	-5.540343	1.600113	1.201044
H	-1.893099	-3.076413	1.556886
H	0.656528	1.132549	-2.282142
H	6.024306	2.945872	1.625848
H	4.490101	3.519994	2.335303
H	5.437267	2.262075	3.149697

TS'1f,3f

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.267323

Total energy: -4927.011073450

Ni	-0.287045	-1.034532	-0.700362
C	3.081587	-0.618229	-0.027182
C	4.455006	-0.755754	-0.056361
C	2.420244	0.197249	0.867726
C	5.202142	-0.030934	0.878295
H	4.955081	-1.405532	-0.785161
C	3.181912	0.913630	1.792832
H	1.321018	0.275213	0.838487
C	4.580207	0.807678	1.813246
H	6.295898	-0.116019	0.880897
H	2.684694	1.573224	2.514962
Br	1.759238	-1.665647	-1.500531
N	-1.972114	-1.222473	0.196229
C	-4.535641	-1.224436	1.354380
C	-2.515710	-2.355074	0.674914
C	-2.692894	-0.064775	0.284909
C	-3.974503	-0.056533	0.858891
C	-3.766451	-2.406602	1.254064
N	-0.817966	0.853243	-0.832209
C	-1.816768	3.474777	-0.734684
C	-0.120074	1.875003	-1.348606
C	-2.024492	1.108263	-0.252398
C	-2.534500	2.416557	-0.196195
C	-0.568237	3.180356	-1.329683
H	-1.901955	-3.258421	0.582466
H	-4.539593	0.879172	0.912300
H	-4.156077	-3.357024	1.630972
H	0.846027	1.618059	-1.801396
H	-3.500732	2.607026	0.281419
H	0.038752	3.976246	-1.771592
C	-2.322400	4.877031	-0.694133
H	-3.303262	4.946214	-0.201180
H	-1.618686	5.535418	-0.156640
H	-2.417651	5.291541	-1.712318
C	-5.893566	-1.253706	1.969622
H	-6.362133	-0.258498	1.977764
H	-6.560007	-1.944297	1.424995
H	-5.848377	-1.622446	3.008690
C	5.386640	1.557131	2.828447
H	6.414495	1.739686	2.478253
H	4.927948	2.527786	3.074955
H	5.464045	0.992014	3.774216

TS'1g,3g

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.204544

Total energy: -4846.456188310

Ni	0.924578	-1.116054	0.096535
N	2.538097	-0.543377	-0.815513
C	2.956947	0.617036	-0.375411
C	3.547640	-1.009122	-1.757478
C	4.438375	0.221545	-1.970323
H	4.102831	-1.862654	-1.328027
H	5.515655	0.012831	-1.916008
N	1.136043	0.626532	1.085537
C	0.446763	1.545089	1.976940
C	2.173733	1.269139	0.623425
C	1.438392	2.707049	2.135269
H	-0.513676	1.863450	1.527554
H	1.971623	2.681532	3.100238
O	4.087775	1.109139	-0.892204
O	2.403351	2.503696	1.083904
H	3.090829	-1.363749	-2.694661
H	4.227452	0.737085	-2.922342
H	0.202388	1.067007	2.939366
H	0.990346	3.702406	2.009136
Br	-1.017864	-2.189575	0.650499
C	-2.484345	-0.626205	-0.097862
C	-3.849685	-0.781513	0.035983
C	-1.897243	0.501601	-0.630652
C	-4.669203	0.265597	-0.398309
H	-4.286886	-1.692924	0.461497
C	-2.731314	1.535933	-1.061853
H	-0.799097	0.569249	-0.704717
C	-4.125008	1.434623	-0.947728
H	-5.758836	0.173020	-0.312253
H	-2.295248	2.442775	-1.498870
C	-5.012472	2.562553	-1.380116
H	-4.557063	3.147621	-2.193854
H	-5.993137	2.199017	-1.723767
H	-5.203572	3.263279	-0.548793

TS'1h,3h

Geometry with 45 atoms:

Thermal correction to Gibbs Free Energy: 0.281041

Total energy: -5095.431734320

C	-3.962192	1.362146	1.239903
C	-2.727268	1.273226	0.600193
N	-2.197226	0.072033	0.297216
C	-2.820928	-1.077178	0.622816
C	-4.058732	-1.054659	1.263149
C	-4.633966	0.181556	1.565920
C	-1.863544	2.395178	0.210611
C	-2.049691	-2.271532	0.256453
C	-2.435739	-3.577784	0.573759
C	-1.608918	-4.634895	0.221661
C	-0.407022	-4.362700	-0.439043
C	-0.096169	-3.041344	-0.728168
N	-0.729753	2.035292	-0.445376
N	-0.889736	-2.015641	-0.402967
C	0.142110	2.988190	-0.790864
C	-0.061264	4.335271	-0.525407
C	-1.235430	4.714614	0.131913
C	-2.143226	3.733461	0.504221
Ni	-0.552783	-0.003016	-0.706700
H	-4.401513	2.332474	1.483844
H	-4.574131	-1.981776	1.525416
H	-5.605847	0.225105	2.062946
H	-3.374302	-3.760534	1.102715
H	-1.892986	-5.661905	0.464635
H	0.277752	-5.162701	-0.728730
H	0.831946	-2.779316	-1.252067
H	1.044574	2.643445	-1.311533
H	0.684502	5.072449	-0.830772
H	-1.435708	5.765271	0.356608
H	-3.062717	4.000036	1.030983
Br	1.440975	-0.093659	-2.063773
C	2.863951	-0.099088	-0.292124
C	4.238197	-0.087111	-0.429498
C	2.226911	-0.101375	0.931379
C	5.011314	-0.075344	0.736019
H	4.717252	-0.090947	-1.416239
C	3.014478	-0.091286	2.084824
H	1.122784	-0.115021	0.984773
C	4.413899	-0.073964	2.004072
H	6.105858	-0.070013	0.661494
H	2.536745	-0.099595	3.072566
C	5.252130	-0.029929	3.246126
H	5.449538	1.009851	3.560138
H	4.752412	-0.529495	4.090409
H	6.231255	-0.509301	3.092855

TS1a',3a'

Geometry with 37 atoms:

Thermal correction to Gibbs Free Energy: 0.222663

Total energy: -7422.557481140

Ni	-0.831124	-0.174980	0.341039
C	0.153985	-1.079535	-1.116702
C	2.810588	-1.810436	-1.649568
C	0.654360	-2.284710	-0.615540
C	0.923052	-0.301772	-1.989056
C	2.247322	-0.657286	-2.220234
C	1.983665	-2.624068	-0.865826
H	0.021848	-2.924846	0.008197
H	0.505392	0.599928	-2.449422
H	2.865791	-0.021823	-2.865218
H	2.388709	-3.547920	-0.436515
N	0.882788	0.516082	1.252891
C	3.369929	1.458884	1.992687
C	1.694293	-0.244226	1.983425
C	1.261515	1.751734	0.888399
C	2.511443	2.258759	1.245789
C	2.957210	0.186476	2.376453
N	-0.813741	1.798212	-0.296726
C	-0.568209	4.461798	-1.014262
C	-1.765549	2.395331	-1.013897
C	0.270211	2.500576	0.086051
C	0.424423	3.842045	-0.263204
C	-1.687037	3.729595	-1.396806
H	1.306038	-1.231404	2.261838
H	2.817867	3.260342	0.937297
H	3.599911	-0.467448	2.969895
H	-2.620788	1.774328	-1.301933
H	1.305813	4.402819	0.054400
H	-2.491039	4.178260	-1.984019
Br	-1.754054	-1.367543	2.229973
Br	-2.065602	-1.106428	-1.543692
C	4.251109	-2.147687	-1.871253
H	-0.466561	5.513230	-1.295308
H	4.357758	1.832195	2.275182
H	4.904576	-1.564434	-1.197527
H	4.455419	-3.212136	-1.677945
H	4.571541	-1.915602	-2.899754

TS1b',3b'

Geometry with 61 atoms:

Thermal correction to Gibbs Free Energy: 0.432813

Total energy: -7736.942463410

Ni	-1.418416	-0.970620	-0.550630
C	-1.895086	-0.398435	1.285656
C	-1.864572	2.004576	2.736443

C	-2.979499	0.481963	1.192391
C	-0.863324	-0.153673	2.195681
C	-0.842230	1.056593	2.885311
C	-2.939885	1.682564	1.895828
H	-3.817539	0.250250	0.526854
H	-0.051883	-0.877375	2.327917
H	-0.003388	1.273112	3.557243
H	-3.765786	2.395590	1.784834
N	-0.415545	0.783570	-0.946848
C	1.018370	3.179613	-0.764990
C	-1.011161	1.948448	-1.196781
C	0.888544	0.767569	-0.639758
C	1.632586	1.944187	-0.546843
C	-0.339704	3.158445	-1.114733
N	0.545125	-1.571235	-0.292483
C	3.279846	-2.107854	0.048813
C	0.975816	-2.807368	-0.056095
C	1.450388	-0.575318	-0.374014
C	2.809030	-0.812763	-0.205445
C	2.319648	-3.120281	0.118420
H	-2.072982	1.896557	-1.466699
H	2.688470	1.886376	-0.278037
H	-0.888960	4.082874	-1.312878
H	0.209840	-3.588236	0.008996
H	3.510721	0.021837	-0.279428
H	2.592710	-4.159651	0.308955
Br	-2.995514	-0.899827	-2.381601
Br	-2.437077	-2.569650	0.985619
C	4.770507	-2.352474	0.232467
C	1.748758	4.504846	-0.604102
C	-1.831136	3.313835	3.459954
C	3.226014	4.311230	-0.283897
H	3.377801	3.775124	0.668057
H	3.752116	3.757016	-1.079632
H	3.714449	5.294811	-0.187238
C	1.629878	5.312873	-1.898254
H	0.582656	5.538972	-2.156274
H	2.158520	6.275204	-1.789946
H	2.081676	4.772626	-2.747916
C	1.093237	5.272180	0.548578
H	1.612535	6.232786	0.707615
H	0.032236	5.494424	0.347727
H	1.147357	4.696454	1.489174
C	5.265854	-1.521160	1.419290
H	5.124186	-0.439751	1.259375
H	4.739333	-1.800221	2.348161
H	6.344067	-1.695398	1.575704
C	5.504228	-1.922285	-1.040807
H	6.587556	-2.098058	-0.927302
H	5.156922	-2.499883	-1.914621
H	5.362618	-0.851834	-1.262467
C	5.077674	-3.820443	0.501787
H	4.761754	-4.469081	-0.332698
H	6.164773	-3.952564	0.629038
H	4.591053	-4.182483	1.423237
H	-2.682781	3.417237	4.154347
H	-0.905900	3.432911	4.044171
H	-1.897529	4.161853	2.756666

TS1c',3c'

Geometry with 45 atoms:

Thermal correction to Gibbs Free Energy: 0.280526

Total energy: -7651.585008890

Ni	-0.031264	-1.209429	-0.536398
C	-0.763201	-1.187694	1.302760
C	-2.527654	0.452936	2.743587
C	-2.141517	-1.409800	1.218281
C	-0.253564	-0.250199	2.207510
C	-1.137248	0.577882	2.892165
C	-3.007954	-0.571288	1.917615
H	-2.531027	-2.195819	0.563150
H	0.827375	-0.132038	2.338648
H	-0.736538	1.348763	3.561101
H	-4.090007	-0.714290	1.812792
N	-0.673474	0.701950	-0.951076
C	-1.490867	3.357285	-0.887855
C	-1.933961	1.030496	-1.216264
C	0.213459	1.675279	-0.670502
C	-0.155028	3.010556	-0.634825
C	-2.401624	2.337929	-1.195281
N	1.724767	-0.139518	-0.291324
C	3.928187	1.531438	0.064559
C	2.932597	-0.639545	-0.037377
C	1.586780	1.201133	-0.382780
C	2.657888	2.061014	-0.207335
C	4.065923	0.140217	0.146546
H	-2.604998	0.197149	-1.459009
H	0.557914	3.803607	-0.399062
H	-3.451796	2.538165	-1.413750
H	3.002714	-1.730494	0.035801
H	2.545319	3.144962	-0.280337
H	5.022689	-0.343116	0.350387
Br	-1.162644	-2.353537	-2.345487
Br	0.497937	-3.030728	1.006031
C	-3.463519	1.397367	3.429114
O	4.917958	2.402820	0.224416
O	-1.796032	4.649399	-0.815359
C	6.218613	1.919540	0.501751

H	6.868674	2.798190	0.597410
H	6.243120	1.350768	1.446509
H	6.594027	1.283212	-0.317323
C	-3.134493	5.049543	-1.034992
H	-3.817040	4.588329	-0.300930
H	-3.163245	6.139539	-0.912221
H	-3.470100	4.795385	-2.054795
H	-4.444424	0.934309	3.619878
H	-3.056425	1.754190	4.388463
H	-3.647470	2.293202	2.807647

TS1d',1d'

Geometry with 43 atoms:

Thermal correction to Gibbs Free Energy: 0.273451

Total energy: -7501.164349420

Ni	-0.760594	-0.414900	0.199551
C	0.486696	-0.803661	-1.342054
C	3.275246	-0.787176	-1.728775
C	1.248475	-1.931291	-1.009372
C	1.092988	0.267342	-2.015818
C	2.473153	0.277620	-2.174189
C	2.631879	-1.898331	-1.169504
H	0.762647	-2.816813	-0.583173
H	0.491695	1.111567	-2.372002
H	2.948511	1.141125	-2.654749
H	3.227756	-2.763070	-0.852947
N	0.875886	0.097058	1.395728
C	3.349505	0.945099	2.298966
C	1.644896	-0.743623	2.100634
C	1.282994	1.360133	1.162057
C	2.527950	1.816258	1.590104
C	2.899839	-0.336883	2.572009
N	-0.816602	1.632481	0.027200
C	-0.454447	4.347349	-0.356158
C	-1.800625	2.358654	-0.524875
C	0.315671	2.228797	0.451958
C	0.533649	3.591817	0.265629
C	-1.636910	3.732658	-0.737319
H	2.860297	2.833562	1.376981
H	3.508405	-1.042428	3.144292
H	1.451750	4.067718	0.613245
H	-2.449201	4.302032	-1.196420
Br	-2.459586	-1.203940	1.749201
Br	-1.563250	-1.321042	-1.971649
C	4.765399	-0.725640	-1.839316
H	4.333104	1.275602	2.643050
H	-0.306127	5.417980	-0.519904
C	1.163597	-2.130539	2.354788
H	0.071425	-2.204010	2.237029
H	1.639540	-2.837576	1.653268
H	1.443302	-2.454083	3.369402
C	-3.069836	1.677834	-0.901849
H	-2.977005	1.192458	-1.887659
H	-3.319698	0.887676	-0.174961
H	-3.894790	2.402438	-0.961154
H	5.214886	-1.730543	-1.868863
H	5.087529	-0.175691	-2.738022
H	5.206185	-0.201657	-0.971150

TS1e',3e'

Geometry with 39 atoms:

Thermal correction to Gibbs Free Energy: 0.235262

Total energy: -7498.758553640

Ni	0.847105	-0.563345	0.379184
C	1.135241	0.718556	-1.097164
C	0.306193	3.320096	-1.745013
C	1.828641	1.815803	-0.577436
C	0.115228	0.905130	-2.035925
C	-0.306623	2.198341	-2.325909
C	1.390775	3.102935	-0.886230
H	2.672175	1.659992	0.103017
H	-0.376575	0.046381	-2.505134
H	-1.136921	2.343878	-3.027026
H	1.908136	3.963214	-0.445575
N	-0.726044	0.503480	1.201904
C	-3.040080	1.878343	1.908546
C	-0.657162	1.584905	1.956268
C	-1.930471	0.067392	0.780558
C	-3.137219	0.717459	1.113282
C	-1.799957	2.312286	2.329754
N	-0.763606	-1.667489	-0.365680
C	-3.147706	-2.779501	-1.296624
C	-0.754158	-2.756270	-1.116813
C	-1.952566	-1.108019	-0.044678
C	-3.187255	-1.619261	-0.496010
C	-1.930377	-3.351498	-1.601316
H	-1.692556	3.205497	2.949053
H	-1.864166	-4.251200	-2.216755
Br	2.235736	-0.626617	2.354019
Br	2.407911	-1.120856	-1.407215
C	-0.191827	4.700974	-2.033447
H	-3.951684	2.418094	2.182916
H	-4.083775	-3.209230	-1.666094
H	0.227253	-3.176814	-1.363599
H	0.344634	1.886217	2.286044
C	-4.399968	-0.945840	-0.133563
C	-4.376131	0.178460	0.635101
H	-5.346465	-1.358152	-0.495832

H	-5.302749	0.693967	0.905198
H	-0.546469	4.798461	-3.072029
H	-1.044981	4.961684	-1.381394
H	0.587646	5.459527	-1.861968

TS1f',3f'

Geometry with 43 atoms:

Thermal correction to Gibbs Free Energy: 0.269239

Total energy: -7501.161645210

Ni	-0.879719	-0.520093	-0.479005
C	-1.174935	0.406077	1.244747
C	-0.413319	2.851440	2.393886
C	-1.929626	1.555793	0.991535
C	-0.126809	0.438658	2.171042
C	0.261306	1.660885	2.709170
C	-1.525693	2.768980	1.547271
H	-2.793771	1.507965	0.320808
H	0.413646	-0.476934	2.433896
H	1.114678	1.694264	3.396875
H	-2.091082	3.678572	1.312576
N	0.618628	0.762398	-1.065400
C	2.749725	2.543036	-1.319146
C	0.415204	1.996148	-1.522611
C	1.862420	0.370488	-0.746082
C	2.948320	1.235227	-0.867449
C	1.445014	2.916063	-1.661074
N	0.799355	-1.654834	-0.054146
C	3.216273	-2.961750	0.474358
C	0.812627	-2.912508	0.389234
C	1.971104	-1.019933	-0.250423
C	3.188361	-1.643597	0.010374
C	1.986258	-3.599498	0.663848
H	-0.619281	2.244047	-1.790193
H	3.956222	0.905287	-0.601673
H	1.234092	3.921945	-2.035313
H	-0.163619	-3.385427	0.543463
H	4.129267	-1.110597	-0.150264
H	1.942333	-4.629360	1.029055
Br	-2.348328	-0.220577	-2.378141
Br	-2.359893	-1.509268	1.194149
C	4.504747	-3.664623	0.729866
C	3.879940	3.510058	-1.410348
H	4.815194	-4.226536	-0.168234
H	4.410479	-4.393952	1.548355
H	5.313458	-2.957962	0.967785
H	3.754063	4.197077	-2.260867
H	4.848871	2.997722	-1.502471
H	3.921871	4.132332	-0.499433
C	0.053303	4.164718	2.937431
H	-0.760014	4.906498	2.966103
H	0.465278	4.063474	3.954232
H	0.856980	4.591823	2.310182

TS1g',3g'

Geometry with 35 atoms:

Thermal correction to Gibbs Free Energy: 0.207244

Total energy: -7420.607236240

C	1.378332	-0.258001	-0.705256
C	3.337213	1.736496	-0.458693
C	2.388002	-0.394258	0.251418
C	1.390860	0.813825	-1.604455
C	2.349184	1.809293	-1.454544
C	3.340721	0.616835	0.380964
H	2.399725	-1.262778	0.917771
H	0.633121	0.889885	-2.391269
H	2.334946	2.671364	-2.132075
H	4.110200	0.529203	1.156936
Br	-0.451711	-2.125181	2.148238
Br	0.594697	-2.189777	-1.540552
C	4.373788	2.808384	-0.335773
H	4.909535	2.748166	0.623957
H	5.129346	2.733038	-1.137889
H	3.928582	3.813519	-0.418422
Ni	-0.314678	-0.734027	0.179925
N	-1.732699	0.202903	-1.056572
C	-2.086793	1.348627	-0.612382
C	-2.454709	-0.003433	-2.306479
C	-3.337995	1.247111	-2.430559
H	-1.736762	-0.107519	-3.137582
H	-3.151448	1.839253	-3.337429
N	-0.603716	1.073447	1.186906
C	-0.166227	1.749527	2.397772
C	-1.473255	1.824022	0.632814
C	-0.955521	3.068864	2.382228
H	-0.387734	1.113975	3.270735
H	-0.322383	3.961985	2.278184
O	-2.966933	2.061827	-1.282447
O	-1.788276	2.976392	1.190452
H	-3.035489	-0.938275	-2.261861
H	-4.414913	1.037022	-2.356148
H	0.925818	1.901460	2.372546
H	-1.621051	3.202074	3.246939

TS1h',3h'

Geometry with 46 atoms:

Thermal correction to Gibbs Free Energy: 0.287855

Total energy: -7669.567387550

C	-1.300214	2.509743	-2.237772

C	-1.213240	1.275260	-1.591164
N	-0.023885	0.748490	-1.295630
C	1.121461	1.364927	-1.590797
C	1.113577	2.602015	-2.238049
C	-0.116903	3.170867	-2.557884
C	-2.363281	0.451014	-1.154242
C	2.331138	0.632051	-1.152171
C	3.629289	1.042951	-1.452662
C	4.697582	0.283711	-0.984949
C	4.441639	-0.867544	-0.246240
C	3.115699	-1.211139	0.004546
N	-2.042939	-0.638491	-0.432426
N	2.095179	-0.475329	-0.424781
C	-3.003465	-1.454287	-0.009181
C	-4.352059	-1.211123	-0.256755
C	-4.695967	-0.077673	-0.987327
C	-3.689274	0.763034	-1.452204
Ni	0.035263	-0.809694	-0.010309
H	-2.266633	2.957606	-2.477251
H	2.042673	3.122411	-2.478250
H	-0.154052	4.142231	-3.056300
H	3.806696	1.941131	-2.047803
H	5.724010	0.588414	-1.203238
H	5.252337	-1.493006	0.132576
H	2.856108	-2.109801	0.576118
H	-2.674649	-2.336618	0.552231
H	-5.112290	-1.899228	0.118071
H	-5.742947	0.149531	-1.202466
H	-3.935518	1.647691	-2.042951
Br	0.112396	-3.158413	-0.997142
C	-0.021986	0.555023	1.625477
C	1.151601	1.317007	1.775736
C	-1.259150	1.207916	1.776719
C	1.078838	2.704703	1.805982
H	2.129433	0.827080	1.816335
C	-1.312696	2.596233	1.806202
H	-2.188457	0.631517	1.818388
C	-0.149967	3.379665	1.776197
H	2.009297	3.283054	1.852573
H	-2.291718	3.087857	1.853240
C	-0.217221	4.872716	1.708802
H	0.653789	5.343635	2.190767
H	-0.230024	5.221173	0.659731
H	-1.129501	5.263328	2.186121
Br	0.063409	-1.429635	2.422886

3f-s

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.274216

Total energy: -4927.092233960

Ni	-0.213487	-0.646473	-0.045620
C	-2.051739	-0.287545	0.010461
C	-2.663408	0.046047	1.226878
C	-2.855232	-0.244275	-1.137495
C	-4.004496	0.432708	1.290617
H	-2.079672	0.027338	2.157772
C	-4.193285	0.149819	-1.078415
H	-2.429563	-0.516404	-2.112630
C	-4.796526	0.496210	0.137914
H	-4.449354	0.697856	2.258588
H	-4.790446	0.188489	-1.998910
Br	-0.720062	-2.899707	-0.080540
C	2.448361	0.296647	0.023096
C	3.837492	0.344446	0.091579
C	4.576960	-0.840878	0.125288
C	3.858502	-2.039434	0.089820
C	2.473217	-2.009691	0.020961
C	1.590470	1.491356	-0.023458
C	2.091750	2.788540	-0.027247
C	1.225811	3.881768	-0.100368
C	-0.139671	3.597617	-0.177872
C	-0.573669	2.281506	-0.162071
H	4.359404	1.304389	0.122699
H	4.378876	-3.001008	0.119444
H	1.878454	-2.929885	-0.006943
H	3.170187	2.958869	0.020427
H	-0.874909	4.403582	-0.252999
H	-1.641164	2.053742	-0.219728
N	1.776052	-0.871390	-0.011835
N	0.261024	1.235834	-0.079212
C	6.065641	-0.823726	0.173378
H	6.479442	-0.853956	-0.849669
H	6.446067	0.091185	0.651394
H	6.461441	-1.700976	0.706751
C	1.736351	5.280067	-0.078272
H	1.772075	5.654364	0.959670
H	2.757325	5.345637	-0.482490
H	1.079209	5.957992	-0.643088
C	-6.241171	0.889900	0.202609
H	-6.552876	1.446430	-0.696390
H	-6.902927	0.007657	0.272689
H	-6.453438	1.518097	1.082601

3f-t

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.269437

Total energy: -4927.074197680

Ni	0.527637	-0.616265	-0.798839

N	-0.881075	0.811618	-1.146239
C	1.840712	0.454476	0.217678
N	-0.855774	-1.149615	0.578135
Br	1.321443	-2.486144	-2.010160
C	-0.771477	1.809038	-2.023510
C	-1.728519	2.806750	-2.136473
C	-2.852492	2.778628	-1.303366
C	-2.944190	1.733346	-0.379120
C	-1.945158	0.765991	-0.322436
C	-1.938391	-0.354336	0.643628
C	-2.951601	-0.589799	1.569856
C	-2.851506	-1.668102	2.452952
C	-1.714123	-2.479399	2.356785
C	-0.745102	-2.185585	1.410148
C	3.198128	0.091944	0.247102
C	4.143687	0.801168	0.991604
C	3.774338	1.916935	1.752590
C	2.424167	2.288198	1.740496
C	1.487785	1.572960	0.990612
C	-3.904127	-1.936153	3.472759
C	-3.920780	3.811519	-1.405761
C	4.789590	2.697492	2.529950
H	0.125235	1.808538	-2.654023
H	-1.597833	3.608554	-2.868397
H	-3.799489	1.687753	0.300522
H	-3.827627	0.063109	1.610404
H	-1.587745	-3.340066	3.019493
H	0.156495	-2.799901	1.304773
H	3.535019	-0.781182	-0.329460
H	5.194232	0.481966	0.988933
H	2.103925	3.154153	2.334524
H	0.441061	1.912391	1.022022
H	-4.104590	-3.014718	3.565476
H	-3.569908	-1.588873	4.465646
H	-4.843713	-1.415776	3.237040
H	-4.695168	3.486020	-2.122091
H	-4.421277	3.973740	-0.439603
H	-3.522867	4.769418	-1.772112
H	4.336680	3.207504	3.395239
H	5.603793	2.053196	2.899323
H	5.261732	3.480194	1.909157

3g-t

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.208507

Total energy: -4846.519923090

Ni	0.254760	0.758882	-0.337622
N	1.449629	-0.002619	1.149593
C	2.049212	-1.076971	0.801181
C	1.904989	0.323157	2.494705
C	2.852650	-0.834699	2.844721
H	2.402606	1.306547	2.487543
H	3.884516	-0.520841	3.055250
N	1.041475	-0.898041	-1.318999
C	0.828624	-1.691304	-2.524657
C	1.772426	-1.603520	-0.540554
C	1.732926	-2.913610	-2.316395
H	-0.241261	-1.952107	-2.600452
H	2.617844	-2.920576	-2.970178
O	2.876495	-1.657159	1.640980
O	2.204570	-2.777272	-0.944351
H	1.045085	0.394970	3.178735
H	2.494292	-1.465789	3.670635
H	1.091071	-1.113505	-3.423464
H	1.215981	-3.878882	-2.401215
C	-1.551450	0.054861	0.011820
C	-2.678994	0.882154	-0.113683
C	-3.974777	0.411046	0.112278
H	-2.547955	1.934897	-0.401016
C	-3.089576	-1.755403	0.617227
C	-4.204754	-0.917891	0.487294
H	-4.831116	1.088208	-0.003390
H	-3.240650	-2.804132	0.904480
C	-5.588708	-1.419675	0.764985
H	-5.861786	-1.287772	1.827493
H	-6.344905	-0.879019	0.173445
H	-5.684603	-2.494920	0.544027
C	-1.798925	-1.276057	0.383576
Br	0.577745	3.086093	-0.503083
H	-0.961565	-1.981472	0.497238

3h-t

Geometry with 45 atoms:

Thermal correction to Gibbs Free Energy: 0.287032

Total energy: -5095.491814370

C	0.562569	-3.224009	-1.874287
C	0.687001	-2.271526	-0.861702
N	-0.383230	-1.598572	-0.432458
C	-1.599912	-1.789977	-0.947195
C	-1.799652	-2.730507	-1.959775
C	-0.699494	-3.449513	-2.418722
C	1.948920	-1.902126	-0.182566
C	-2.645473	-0.912748	-0.374808
C	-3.981920	-0.949031	-0.771779
C	-4.879778	-0.063372	-0.184529
C	-4.420860	0.832355	0.776717
C	-3.071401	0.804902	1.117282
N	1.830452	-0.956522	0.768852

N	-2.212987	-0.044840	0.559453
C	2.908730	-0.556125	1.437125
C	4.175814	-1.078266	1.190481
C	4.310332	-2.053938	0.207732
C	3.182403	-2.475334	-0.489780
Ni	-0.095176	-0.023426	0.801213
H	1.428248	-3.781745	-2.236186
H	-2.789226	-2.898687	-2.388743
H	-0.825408	-4.189982	-3.211794
H	-4.319769	-1.658212	-1.530120
H	-5.931922	-0.073759	-0.479211
H	-5.093999	1.544116	1.258706
H	-2.649861	1.482271	1.870043
H	2.737542	0.210277	2.203169
H	5.036052	-0.723426	1.761602
H	5.287557	-2.488268	-0.016680
H	3.264818	-3.241049	-1.263881
C	0.342338	1.310647	-0.620027
C	1.244592	2.351856	-0.346062
C	-0.154512	1.262639	-1.930582
C	1.622287	3.286294	-1.312197
H	1.672044	2.444610	0.663008
C	0.214686	2.193265	-2.905950
H	-0.858184	0.469875	-2.230176
C	1.110284	3.227465	-2.614246
H	2.333927	4.082012	-1.054738
H	-0.197857	2.114281	-3.920380
Br	0.025097	1.017391	3.025667
C	1.490433	4.247968	-3.645293
H	0.860280	5.152460	-3.575403
H	2.533900	4.580445	-3.523372
H	1.374438	3.856036	-4.668105

3f'-s

Geometry with 43 atoms:

Thermal correction to Gibbs Free Energy: 0.27163

Total energy: -7501.168182150

C	-1.606912	1.225635	-0.150035
C	-2.412780	2.341564	-0.364922
C	-2.168310	3.181936	-1.453576
C	-1.097391	2.854916	-2.295226
C	-0.335080	1.730830	-2.024256
C	-1.792690	0.266114	0.957025
C	-2.780575	0.374468	1.931801
C	-2.879571	-0.598142	2.931718
C	-1.966973	-1.658466	2.895289
C	-1.006025	-1.700514	1.894987
H	-3.240690	2.562166	0.314205
H	-0.859121	3.477164	-3.162145
H	0.506231	1.443449	-2.664791
H	-3.481871	1.213157	1.920262
H	-2.007191	-2.452155	3.646502
H	-0.269536	-2.510530	1.833815
N	-0.586267	0.945801	-0.977740
N	-0.923690	-0.757665	0.959856
Ni	0.407696	-0.712007	-0.566172
C	-3.906302	-0.497194	4.006560
C	-3.023765	4.370116	-1.727371
C	1.711553	0.409300	0.310784
C	1.696697	0.767305	1.653262
C	2.661003	0.963886	-0.545997
C	2.628096	1.695896	2.130496
H	0.968930	0.339335	2.351801
C	3.581719	1.891834	-0.060261
H	2.695275	0.676350	-1.605671
C	3.582273	2.274062	1.288188
H	2.606578	1.978240	3.190027
H	4.320767	2.328030	-0.743355
Br	1.913329	-2.461935	-0.168528
Br	-0.978811	-1.895217	-2.160048
H	-4.779674	0.086609	3.680751
H	-4.240432	-1.491806	4.337908
H	-3.482838	0.011451	4.890000
H	-3.647666	4.633830	-0.861491
H	-2.413583	5.242443	-2.008748
H	-3.696545	4.167033	-2.578227
C	4.591199	3.252481	1.806025
H	4.295274	3.662911	2.783873
H	5.581110	2.780569	1.936500
H	4.734064	4.095157	1.109972

3g'-s

Geometry with 35 atoms:

Thermal correction to Gibbs Free Energy: 0.208418

Total energy: -7420.612319580

Ni	0.301879	-0.546764	-0.329048
N	0.961254	0.354435	1.402427
C	1.195989	1.599023	1.237639
C	1.450679	-0.005719	2.723700
C	1.900656	1.343904	3.312459
H	2.271821	-0.734659	2.614533
H	2.951870	1.369301	3.627529
N	0.412658	1.351988	-0.956761
C	0.235621	2.101154	-2.191802
C	0.872442	2.160034	-0.077632
C	0.612815	3.536607	-1.784255
H	-0.802469	2.012633	-2.549446
H	1.438703	3.964807	-2.367016

O	1.744961	2.286321	2.211559
O	1.061879	3.415286	-0.403867
H	0.656986	-0.495132	3.310878
H	1.267592	1.696274	4.138942
H	0.895988	1.677751	-2.966771
H	-0.235803	4.234619	-1.793734
Br	2.537060	-0.953065	-1.243612
Br	-0.137898	-2.742095	0.335842
C	-1.584046	-0.249830	-0.058232
C	-2.169694	0.076217	1.156650
C	-2.330653	-0.280088	-1.230293
C	-3.528581	0.397222	1.186848
H	-1.589575	0.079216	2.085077
C	-3.688897	0.041484	-1.181925
H	-1.867630	-0.548992	-2.188975
C	-4.309324	0.384363	0.025106
H	-3.994087	0.661884	2.143386
H	-4.278076	0.027004	-2.106077
C	-5.773763	0.697998	0.077630
H	-6.371160	-0.210010	0.270340
H	-6.132150	1.121838	-0.872937
H	-6.006860	1.411384	0.883007

3h'-s

Geometry with 46 atoms:

Thermal correction to Gibbs Free Energy: 0.288445

Total energy: -7669.584285190

C	1.500718	-0.298825	3.439183
C	1.387592	-0.197298	2.052077
N	0.229749	-0.482390	1.453516
C	-0.843207	-0.908281	2.121683
C	-0.799917	-1.025966	3.511679
C	0.386118	-0.707118	4.166442
C	2.473779	0.197835	1.129091
C	-1.992228	-1.273149	1.265252
C	-3.189728	-1.788523	1.760087
C	-4.180787	-2.161231	0.857522
C	-3.947014	-2.020586	-0.507022
C	-2.728034	-1.489044	-0.919182
N	2.126344	0.253239	-0.168441
N	-1.790918	-1.117794	-0.053506
C	3.022368	0.597996	-1.085518
C	4.335799	0.919260	-0.750430
C	4.709363	0.870785	0.588542
C	3.768079	0.502772	1.545997
Ni	0.107908	-0.288629	-0.516555
H	2.438649	-0.066593	3.946433
H	-1.670501	-1.365682	4.075283
H	0.446070	-0.788144	5.253893
H	-3.346448	-1.904773	2.834230
H	-5.127876	-2.566853	1.221073
H	-4.695082	-2.313655	-1.245987
H	-2.487344	-1.343809	-1.980103
H	2.663661	0.621183	-2.122044
H	5.045966	1.203078	-1.529370
H	5.729758	1.117555	0.891184
H	4.041164	0.456077	2.601935
Br	0.923240	-2.625701	-0.781111
C	-0.566216	1.546852	-0.251878
C	-1.902170	1.846747	-0.529315
C	0.248162	2.557290	0.257111
C	-2.413090	3.117835	-0.272033
H	-2.569392	1.102621	-0.971588
C	-0.273398	3.830315	0.508429
H	1.307656	2.397013	0.472600
C	-1.612105	4.135408	0.258500
H	-3.465039	3.324854	-0.502212
H	0.390818	4.604647	0.910064
C	-2.177632	5.490284	0.555890
H	-2.907990	5.800818	-0.207913
H	-2.707393	5.500771	1.524285
H	-1.389454	6.256596	0.609454
Br	-0.063628	0.140397	-2.880355

4

Geometry with 22 atoms:

Thermal correction to Gibbs Free Energy: 0.148079

Total energy: -404.709975020

N	-2.084025	0.079531	-0.001068
C	-0.693210	0.047882	-0.009817
C	0.009967	-1.170840	0.081946
C	0.065696	1.232762	-0.116106
C	1.400040	-1.189900	0.081750
H	-0.527902	-2.117966	0.165815
C	1.454507	1.188182	-0.112897
H	-0.435641	2.196555	-0.235830
C	2.159988	-0.017101	-0.007842
H	1.914174	-2.155412	0.156948
H	2.012888	2.127182	-0.207525
C	3.656195	-0.047892	0.028928
H	4.041398	0.020762	1.062545
H	4.054790	-0.982824	-0.396540
H	4.093912	0.795429	-0.529008
C	-2.814702	-1.162108	-0.148785
H	-3.875372	-0.938808	-0.321764
H	-2.441207	-1.745185	-1.006004
H	-2.741438	-1.793491	0.754883
C	-2.792416	1.245159	0.168502

H -2.303127 2.104280 0.631565
H -3.880683 1.175901 0.138323

TS3f,1f'
Geometry with 64 atoms:
Thermal correction to Gibbs Free Energy: 0.444749
Total energy: -5331.792366910
Ni -0.944486 -0.951553 -0.820835
C -0.610378 -0.803527 1.146551
C -1.156376 -0.034403 3.877334
C -1.530118 -1.513672 1.975900
C -0.083588 0.384311 1.727273
C -0.320176 0.734018 3.055052
C -1.774514 -1.159583 3.292677
H -2.036127 -2.400491 1.565726
H 0.570545 1.040528 1.136267
H 0.140918 1.642070 3.466198
H -2.475634 -1.752146 3.895730
N 0.103408 0.666818 -1.425085
C 1.473771 3.105319 -1.547130
C 1.400957 0.706928 -1.746705
C -0.549756 1.827751 -1.183925
C 0.117056 3.056401 -1.239216
C 2.119506 1.885637 -1.820131
N -2.422760 0.407802 -0.836983
C -4.166910 2.509825 -0.264137
C -3.699578 0.161785 -0.528828
C -1.973875 1.681542 -0.857303
C -2.830745 2.749758 -0.576430
C -4.599663 1.172122 -0.242108
H 1.882559 -0.253615 -1.955787
H -0.423392 3.983946 -1.030893
H 3.180390 1.861982 -2.088389
H -3.998884 -0.893221 -0.517569
H -2.456157 3.776979 -0.594941
H -5.638490 0.928550 -0.001369
Br -1.756024 -3.044123 -1.593235
C 1.044875 -2.276048 1.183964
C -5.113656 3.619432 0.042102
H -4.624999 4.602913 -0.010963
H -5.962548 3.614551 -0.661923
H -5.544164 3.498760 1.050189
C 2.229377 4.388633 -1.592134
H 1.591967 5.251329 -1.350747
H 3.071565 4.367682 -0.879752
H 2.670316 4.549282 -2.590190
C -1.402488 0.320582 5.309728
H -1.069115 1.345312 5.539035
H -2.471927 0.244503 5.571679
H -0.866520 -0.356281 6.000404
H 1.320036 -2.027687 2.214831
H 0.413431 -3.161811 1.071989
N 2.037854 -2.169398 0.233636
C 3.088421 -1.258383 0.342874
C 3.176604 -0.354249 1.421160
C 4.099061 -1.197569 -0.637356
C 4.215147 0.565727 1.495856
H 2.417249 -0.353888 2.205753
C 5.129780 -0.267542 -0.542549
H 4.089378 -1.879675 -1.490159
C 5.213754 0.642632 0.516649
H 4.246200 1.255873 2.347324
H 5.896887 -0.250078 -1.325662
C 1.953807 -2.996382 -0.953732
H 1.048725 -3.614784 -0.903558
H 1.889283 -2.391707 -1.876581
H 2.831640 -3.659418 -1.043368
C 6.291089 1.679173 0.580713
H 5.958565 2.636593 0.138889
H 6.586445 1.897043 1.619820
H 7.190503 1.366837 0.026752

TS3g,1g'
Geometry with 56 atoms:
Thermal correction to Gibbs Free Energy: 0.380843
Total energy: -5251.241552200
Ni 1.200881 -0.921961 0.260096
N 2.593830 0.152229 1.217348
C 1.999490 0.929903 2.097769
C 3.794775 0.853364 0.808684
C 4.003811 1.850815 1.949518
H 4.652396 0.176048 0.672390
H 4.690020 1.462241 2.722083
N 0.030901 -0.340320 1.833314
C -1.358977 -0.249674 2.251339
C 0.655657 0.648496 2.445432
C -1.292789 0.647195 3.488140
H -1.979927 0.205793 1.450389
H -1.241961 0.064532 4.424596
O 2.695256 1.989183 2.536014
O -0.055161 1.361466 3.332123
H 3.617967 1.363127 -0.163131
H 4.351929 2.842987 1.631839
H -1.797352 -1.235919 2.474006
H -2.112709 1.373852 3.566452
C 0.763218 0.508305 -1.057402
C 1.556559 0.623289 -2.216917
C 1.629662 1.806454 -2.944285

H	2.120655	-0.251136	-2.569644
C	0.140648	2.854740	-1.386926
C	0.915354	2.948462	-2.546972
H	2.252415	1.854413	-3.846519
H	-0.424544	3.732074	-1.048500
C	1.007351	4.221183	-3.331012
H	1.978319	4.722859	-3.173609
H	0.922815	4.036935	-4.414514
H	0.220305	4.934821	-3.043428
C	0.074769	1.666680	-0.654443
Br	2.309391	-2.775715	-0.838825
H	-0.552538	1.651153	0.246315
N	-1.774205	-1.670701	-1.146951
C	-2.927439	-0.945337	-0.766609
C	-3.947513	-1.567070	-0.032532
C	-3.061539	0.417212	-1.076361
C	-5.060573	-0.841179	0.376754
H	-3.885633	-2.623448	0.233853
C	-4.182302	1.124027	-0.660366
H	-2.273960	0.951423	-1.611808
C	-5.207915	0.516240	0.073519
H	-5.839668	-1.349916	0.954301
H	-4.254723	2.189361	-0.904301
C	-6.419779	1.283719	0.498419
H	-7.203195	1.255106	-0.278856
H	-6.862218	0.867184	1.416048
H	-6.184862	2.344230	0.676851
C	-1.581081	-3.007444	-0.597726
H	-0.586432	-3.372517	-0.885217
H	-1.639569	-2.989776	0.501816
H	-2.345843	-3.698805	-0.983135
C	-0.841172	-1.159614	-1.953797
H	-1.094159	-0.303195	-2.577320
H	-0.016650	-1.810722	-2.251210

TS3h,1h'

Geometry with 67 atoms:

Thermal correction to Gibbs Free Energy: 0.462644

Total energy: -5500.211508560

C	-0.983311	-2.726718	-1.987058
C	-0.757633	-1.372958	-1.741262
N	0.497815	-0.907475	-1.591508
C	1.568603	-1.718706	-1.663171
C	1.409144	-3.077691	-1.925562
C	0.116183	-3.582324	-2.084976
C	-1.784634	-0.330174	-1.659577
C	2.847679	-1.031662	-1.432748
C	4.089188	-1.674507	-1.433429
C	5.234303	-0.930347	-1.183269
C	5.117326	0.440430	-0.941735
C	3.848491	1.005753	-0.953993
N	-1.329071	0.886927	-1.277487
N	2.745968	0.295436	-1.191983
C	-2.158392	1.930884	-1.313552
C	-3.492307	1.822494	-1.684174
C	-3.983698	0.559971	-2.032329
C	-3.122098	-0.524473	-2.026802
Ni	0.742705	0.844906	-0.667764
H	-1.999093	-3.113477	-2.100004
H	2.273824	-3.740972	-1.999193
H	-0.034919	-4.646490	-2.279928
H	4.156430	-2.748405	-1.622231
H	6.213542	-1.415772	-1.175142
H	5.993857	1.060737	-0.743523
H	3.692655	2.073342	-0.753337
H	-1.714647	2.894169	-1.031440
H	-4.131191	2.708294	-1.700783
H	-5.031403	0.427647	-2.316370
H	-3.475022	-1.516307	-2.321093
C	1.131714	-0.041864	1.170034
C	2.186685	0.579797	1.890180
C	1.076363	-1.449877	1.319378
C	3.071571	-0.122730	2.694213
H	2.308121	1.669511	1.806162
C	1.950171	-2.162655	2.139749
H	0.317444	-2.030368	0.776853
C	2.972428	-1.518473	2.844901
H	3.873235	0.413723	3.218920
H	1.848632	-3.252735	2.220395
Br	1.027064	3.275091	-0.339059
C	3.925089	-2.267039	3.723991
H	4.974275	-2.018028	3.489939
H	3.778770	-2.020118	4.790528
H	3.804926	-3.356390	3.619421
N	-1.805828	1.160062	1.986748
C	-2.814914	0.245349	1.658324
C	-4.153533	0.655578	1.527120
C	-2.514630	-1.111450	1.448678
C	-5.135355	-0.255531	1.159578
H	-4.439071	1.692237	1.719738
C	-3.512450	-2.007099	1.083769
H	-1.485495	-1.464310	1.542991
C	-4.839067	-1.600438	0.908054
H	-6.169537	0.092845	1.058248
H	-3.243276	-3.055497	0.908834
C	-5.890313	-2.551775	0.427589
H	-5.660228	-3.591045	0.709131
H	-6.884756	-2.298188	0.827140

H	-5.973676	-2.528395	-0.674415
C	-2.071676	2.585297	1.898394
H	-1.122406	3.117593	1.740477
H	-2.725406	2.808500	1.044422
H	-2.558686	2.962052	2.814867
C	-0.594227	0.761052	2.452122
H	-0.551054	-0.189074	2.990307
H	0.038796	1.566024	2.828526

TS3h,5h

Geometry with 67 atoms:

Thermal correction to Gibbs Free Energy: 0.461545

Total energy: -5500.222847540

C	-3.709309	1.261718	2.699879
C	-2.938174	1.235417	1.536650
N	-2.702303	0.081226	0.908424
C	-3.164209	-1.085650	1.363519
C	-3.944503	-1.134167	2.520164
C	-4.216520	0.058797	3.184446
C	-2.313158	2.413307	0.895161
C	-2.751655	-2.256229	0.557995
C	-3.096095	-3.570335	0.875809
C	-2.623422	-4.600131	0.068852
C	-1.832341	-4.292265	-1.034500
C	-1.541173	-2.954664	-1.286804
N	-1.637972	2.152311	-0.238408
N	-1.983242	-1.970910	-0.508823
C	-1.052665	3.144897	-0.901966
C	-1.088017	4.463271	-0.456119
C	-1.769706	4.742854	0.724709
C	-2.398117	3.707329	1.409287
Ni	-1.345198	0.061815	-0.588202
H	-3.913704	2.198363	3.221824
H	-4.332232	-2.080717	2.901343
H	-4.825231	0.050471	4.091357
H	-3.719574	-3.789848	1.744921
H	-2.874240	-5.637828	0.301773
H	-1.445904	-5.072256	-1.693373
H	-0.933931	-2.651422	-2.147863
H	-0.538752	2.863668	-1.829728
H	-0.590118	5.249896	-1.026346
H	-1.817518	5.763597	1.111655
H	-2.944691	3.906795	2.333332
C	0.202669	-0.122746	0.684978
C	1.015334	0.967866	1.034399
C	0.530620	-1.336969	1.317811
C	2.094079	0.856742	1.916806
H	0.823608	1.962873	0.605712
C	1.600325	-1.459125	2.205582
H	-0.053437	-2.246219	1.113504
C	2.415100	-0.363075	2.515544
H	2.708028	1.739624	2.138590
H	1.819144	-2.433304	2.663160
C	3.605804	-0.514907	3.413259
H	4.401937	-1.099072	2.916514
H	4.040239	0.461267	3.682400
H	3.356436	-1.046738	4.346736
C	1.758341	-1.139211	-2.145660
H	0.889937	-1.011858	-2.792866
H	1.894378	-2.032714	-1.536639
N	2.560095	-0.045072	-1.935515
C	3.720478	-0.094374	-1.171351
C	4.284481	-1.323373	-0.769496
C	4.381238	1.084296	-0.767554
C	5.428676	-1.357409	0.019092
H	3.837149	-2.265728	-1.093731
C	5.526458	1.025961	0.016570
H	3.987550	2.063719	-1.047668
C	6.075810	-0.190439	0.441613
H	5.839809	-2.331404	0.310500
H	6.008417	1.964108	0.316514
C	7.283509	-0.233657	1.326905
H	7.019101	-0.069737	2.387437
H	7.793718	-1.207936	1.270414
H	8.012981	0.548247	1.060467
C	2.101413	1.234110	-2.431670
H	1.254169	1.075909	-3.112804
H	1.750007	1.880491	-1.604911
H	2.900538	1.766030	-2.972565
Br	-1.652856	0.263457	-3.067235

5a-s

Geometry with 58 atoms:

Thermal correction to Gibbs Free Energy: 0.399823

Total energy: -5253.233676660

C	0.675879	-0.392575	-1.976993
C	-3.279551	0.051629	-0.017568
C	-4.593324	0.421546	-0.309342
C	-4.988263	0.516267	-1.639020
C	-4.069637	0.226218	-2.643042
C	-2.777326	-0.128351	-2.270661
C	-2.767778	-0.118354	1.359094
C	-3.543077	0.055274	2.507141
C	-2.961199	-0.167409	3.750336
C	-1.628208	-0.563670	3.821104
C	-0.922272	-0.710704	2.632334
H	-5.304157	0.632327	0.491585
H	-4.342132	0.274172	-3.698859

H	-2.020656	-0.365239	-3.027328
H	-4.589888	0.356172	2.436108
H	-1.140200	-0.756258	4.778300
H	0.129601	-1.023695	2.623202
N	-2.393621	-0.197777	-0.998412
N	-1.481183	-0.487163	1.446985
Br	-0.636226	-2.995943	-0.384591
Ni	-0.451760	-0.529314	-0.330043
C	0.040474	1.312982	-0.068994
C	-0.644424	2.394668	-0.626646
C	1.095550	1.591212	0.809040
C	-0.288171	3.710301	-0.317245
H	-1.470383	2.231158	-1.331251
C	1.450469	2.905129	1.116115
H	1.676112	0.774210	1.258646
H	-0.838718	4.540582	-0.776475
H	2.285152	3.092973	1.802987
C	0.762465	3.991568	0.561362
C	1.127874	5.401269	0.916696
H	0.753468	-1.468219	-2.209280
H	0.034331	0.099618	-2.723490
N	1.947218	0.236861	-1.971685
C	2.082358	1.549884	-2.555080
H	2.977659	1.609959	-3.198336
H	1.208241	1.761621	-3.184391
H	2.155820	2.348653	-1.792046
C	2.952739	-0.222201	-1.135167
C	4.138582	0.514959	-0.937092
C	2.817006	-1.429798	-0.418261
C	5.118044	0.070112	-0.055353
H	4.295126	1.463235	-1.455262
C	3.809535	-1.851477	0.460043
H	1.918040	-2.043462	-0.523474
C	4.983046	-1.118801	0.669177
H	6.019064	0.679912	0.081359
H	3.658817	-2.788472	1.009794
C	6.052534	-1.597813	1.603104
H	5.630584	-2.177926	2.439166
H	6.778562	-2.256415	1.093781
H	6.626860	-0.758931	2.027034
H	0.640668	5.722214	1.854239
H	2.213044	5.513202	1.069420
H	0.817507	6.110972	0.134210
H	-3.550696	-0.036114	4.660841
H	-6.011486	0.807913	-1.887291

5b-s

Geometry with 82 atoms:

Thermal correction to Gibbs Free Energy: 0.608303

Total energy: -5567.617805750

C	-1.961465	-2.056640	-0.577051
C	2.169333	-0.498132	-0.322265
C	3.467135	-0.944128	-0.095789
C	3.776204	-2.308212	-0.165036
C	2.726174	-3.171367	-0.488483
C	1.451682	-2.654603	-0.695773
C	1.782274	0.929599	-0.293505
C	2.673311	1.972609	-0.060764
C	2.231877	3.301797	-0.075924
C	0.875710	3.512190	-0.343461
C	0.043038	2.420516	-0.563133
H	4.249955	-0.219099	0.138950
H	2.876189	-4.247947	-0.580181
H	0.619045	-3.321504	-0.947837
H	3.725397	1.750172	0.132750
H	0.448839	4.515290	-0.383327
H	-1.025010	2.555973	-0.776180
N	1.172580	-1.359414	-0.600541
N	0.483612	1.169357	-0.533018
Br	-0.792724	-0.271244	-3.125717
Ni	-0.717469	-0.493656	-0.662224
C	-1.009749	-0.396304	1.236370
C	-0.250485	-1.084124	2.185538
C	-1.980206	0.500187	1.700773
C	-0.453097	-0.881932	3.553745
H	0.514380	-1.807789	1.873800
C	-2.180999	0.700799	3.066859
H	-2.614156	1.049521	0.991390
H	0.152383	-1.441499	4.277439
H	-2.951296	1.406200	3.402713
C	-1.417799	0.015776	4.021000
C	-1.616053	0.256220	5.487367
H	-2.167507	-2.162338	-1.655680
H	-1.330327	-2.892474	-0.239103
N	-3.158323	-2.045441	0.183925
C	-3.199544	-2.753164	1.440786
H	-4.094145	-3.397277	1.509867
H	-2.317109	-3.400364	1.524559
H	-3.204743	-2.069256	2.311163
C	-4.168841	-1.141171	-0.100618
C	-5.291837	-1.005397	0.742056
C	-4.103900	-0.296793	-1.229468
C	-6.284551	-0.071108	0.465116
H	-5.390517	-1.621970	1.637837
C	-5.107965	0.631339	-1.482559
H	-3.247323	-0.340635	-1.908335
C	-6.223739	0.771423	-0.649700
H	-7.136583	0.010172	1.150556

H	-5.013479	1.278641	-2.362859
C	-7.310190	1.758600	-0.950845
H	-6.916730	2.651321	-1.462593
H	-8.084385	1.329168	-1.611565
H	-7.822591	2.090304	-0.033958
H	-1.045483	1.135518	5.834783
H	-2.673491	0.449861	5.727827
H	-1.280201	-0.602677	6.088915
C	3.215976	4.433316	0.187425
C	2.539234	5.798965	0.137544
H	3.284164	6.586569	0.334633
H	2.096083	6.004087	-0.851137
H	1.747658	5.894808	0.899295
C	3.830536	4.242528	1.577935
H	4.381486	3.292337	1.665196
H	4.541181	5.058889	1.789149
H	3.052548	4.257413	2.359569
C	4.316161	4.392913	-0.878238
H	3.892747	4.519410	-1.888725
H	5.035557	5.210725	-0.705628
H	4.879545	3.446134	-0.862183
C	5.197225	-2.782561	0.103537
C	5.326215	-4.296035	-0.029670
H	5.073375	-4.643588	-1.045165
H	6.367048	-4.596059	0.172046
H	4.683630	-4.829704	0.690213
C	6.143403	-2.119505	-0.902714
H	5.871428	-2.386708	-1.937577
H	6.136936	-1.020701	-0.822121
H	7.177189	-2.459086	-0.723959
C	5.589170	-2.380418	1.529260
H	5.564442	-1.288794	1.676979
H	4.912989	-2.839465	2.269885
H	6.614829	-2.722294	1.746528

5c-s

Geometry with 66 atoms:

Thermal correction to Gibbs Free Energy: 0.458116

Total energy: -5482.260290320

C	-1.216220	-2.072590	-0.697745
C	2.735689	-0.142380	-0.161048
C	4.062146	-0.454828	0.089531
C	4.495027	-1.782032	-0.045169
C	3.564040	-2.748251	-0.447050
C	2.255403	-2.339494	-0.668419
C	2.203113	1.236936	-0.083582
C	2.974968	2.340104	0.246942
C	2.382737	3.611450	0.262894
C	1.025337	3.723479	-0.067557
C	0.334739	2.560555	-0.381043
H	4.791299	0.301926	0.385273
H	3.830180	-3.796224	-0.588869
H	1.503999	-3.072806	-0.983928
H	4.035092	2.258155	0.494783
H	0.504032	4.681286	-0.084397
H	-0.729618	2.598963	-0.646504
N	1.840329	-1.085559	-0.519624
N	0.898191	1.358140	-0.385258
Br	-0.071670	-0.084454	-3.109673
Ni	-0.119261	-0.403786	-0.648420
C	-0.518906	-0.424647	1.232058
C	0.219130	-1.138137	2.178738
C	-1.550767	0.401355	1.694892
C	-0.063414	-1.030208	3.543263
H	1.030632	-1.807862	1.864907
C	-1.832906	0.506048	3.057462
H	-2.168367	0.970756	0.986987
H	0.528160	-1.607716	4.264328
H	-2.651040	1.156248	3.391729
C	-1.091667	-0.205315	4.009471
C	-1.378402	-0.066374	5.474370
H	-1.344119	-2.153595	-1.790930
H	-0.543147	-2.869895	-0.347493
N	-2.457444	-2.182177	-0.014827
C	-2.524848	-2.962578	1.196950
H	-3.421548	-3.606548	1.207311
H	-1.647095	-3.619087	1.257818
H	-2.545446	-2.333445	2.107995
C	-3.481671	-1.288618	-0.283941
C	-4.629137	-1.212312	0.532573
C	-3.400497	-0.388365	-1.367446
C	-5.623915	-0.273037	0.281099
H	-4.741547	-1.873830	1.394004
C	-4.407280	0.543420	-1.596129
H	-2.531973	-0.391425	-2.031760
C	-5.542949	0.630839	-0.783503
H	-6.493275	-0.236013	0.948427
H	-4.298873	1.235499	-2.440102
C	-6.630174	1.625680	-1.055288
H	-6.232817	2.546515	-1.511125
H	-7.387747	1.226847	-1.753384
H	-7.163529	1.905523	-0.133023
H	-0.873794	0.816683	5.904467
H	-2.455669	0.059578	5.667132
H	-1.029791	-0.943402	6.041505
O	3.170773	4.631315	0.591990
O	5.776203	-2.021700	0.215032
C	2.631671	5.936936	0.624952

H	3.446570	6.607993	0.920130
H	2.256657	6.240596	-0.366547
H	1.816009	6.014760	1.362914
C	6.270329	-3.340030	0.090421
H	6.164946	-3.710532	-0.942710
H	7.334279	-3.304774	0.351452
H	5.752513	-4.027670	0.779565

5d-s

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.453444

Total energy: -5331.846634240

C	0.699619	-0.229658	-2.039824
C	-3.139387	-0.107076	0.454210
C	-4.485778	0.252963	0.436281
C	-5.166059	0.242070	-0.775422
C	-4.492693	-0.152936	-1.920740
C	-3.136927	-0.493185	-1.842444
C	-2.365884	-0.190955	1.713807
C	-2.912011	0.119267	2.959265
C	-2.123410	-0.045392	4.091699
C	-0.830327	-0.531530	3.954689
C	-0.336218	-0.819525	2.678560
H	-5.005683	0.528005	1.354645
H	-5.001584	-0.203207	-2.886372
H	-3.935910	0.483128	3.051984
H	-0.192495	-0.693417	4.826960
N	-2.481513	-0.439465	-0.674254
N	-1.101277	-0.625918	1.594560
Br	-0.339100	-3.036099	-0.566428
Ni	-0.390549	-0.550025	-0.359832
C	-0.181007	1.362459	-0.184801
C	-1.047785	2.279644	-0.785678
C	0.823836	1.872338	0.645776
C	-0.924710	3.651816	-0.553935
H	-1.841468	1.938697	-1.463131
C	0.945285	3.242764	0.878539
H	1.553811	1.202396	1.117029
H	-1.617863	4.345276	-1.045647
H	1.743795	3.609297	1.535325
C	0.068691	4.160830	0.287939
C	0.180694	5.629404	0.565253
H	0.885657	-1.286490	-2.294267
H	0.013501	0.212489	-2.772073
N	1.898315	0.523815	-2.011064
C	1.907876	1.855168	-2.568524
H	2.784909	2.004828	-3.222400
H	1.008154	2.001005	-3.179941
H	1.923040	2.642718	-1.790839
C	2.968764	0.123397	-1.226942
C	4.077621	0.968244	-1.009235
C	2.984748	-1.136901	-0.594711
C	5.132309	0.567752	-0.196338
H	4.114272	1.962154	-1.459891
C	4.051399	-1.513592	0.214880
H	2.147665	-1.831186	-0.710287
C	5.151169	-0.679047	0.438488
H	5.969498	1.258825	-0.042037
H	4.017433	-2.496565	0.701129
C	6.302696	-1.106872	1.296457
H	5.984785	-1.816009	2.077008
H	7.088514	-1.612272	0.707209
H	6.781025	-0.247213	1.792089
H	-0.374799	5.912644	1.476612
H	1.227143	5.934212	0.723928
H	-0.230161	6.231183	-0.260259
H	-6.220987	0.523401	-0.817998
H	-2.523999	0.195551	5.079367
C	1.033437	-1.371796	2.481033
H	0.975426	-2.335058	1.946259
H	1.652906	-0.713093	1.848473
H	1.550969	-1.515164	3.438863
C	-2.397368	-0.909046	-3.068147
H	-1.875158	-0.048293	-3.519385
H	-1.647950	-1.678998	-2.830549
H	-3.090721	-1.297341	-3.827035

5e-s

Geometry with 60 atoms:

Thermal correction to Gibbs Free Energy: 0.41154

Total energy: -5329.434422870

C	-1.087935	-0.488992	1.838733
C	3.045310	-0.149600	0.403480
C	4.381501	0.049106	0.813874
C	4.638971	0.025461	2.199864
C	3.600031	-0.196249	3.078980
C	2.303796	-0.381749	2.569760
C	2.728465	-0.152508	-0.997837
C	3.749050	0.045180	-1.952714
C	3.370087	0.017281	-3.311007
C	2.049546	-0.201917	-3.645987
C	1.108310	-0.387328	-2.619493
H	3.765475	-0.228872	4.157351
H	1.726992	-0.233276	-4.688381
N	2.033461	-0.350162	1.276844
N	1.443253	-0.359981	-1.343781
Br	0.251646	-2.988989	0.088243
Ni	0.179824	-0.529022	0.295790

C	-0.260390	1.330014	0.116924
C	0.429939	2.371113	0.739466
C	-1.273532	1.663432	-0.790623
C	0.117219	3.705549	0.464103
H	1.223935	2.157543	1.467202
C	-1.583144	2.995695	-1.065378
H	-1.854441	0.873662	-1.287163
H	0.668774	4.505897	0.972698
H	-2.384110	3.230413	-1.777446
C	-0.890298	4.043452	-0.444865
C	-1.206070	5.473647	-0.764709
H	-1.217170	-1.576771	1.966937
H	-0.480711	-0.087320	2.663725
N	-2.331664	0.184936	1.811042
C	-2.449119	1.469560	2.458321
H	-3.326174	1.502548	3.128796
H	-1.555854	1.653952	3.068618
H	-2.543102	2.300015	1.732839
C	-3.346146	-0.224727	0.959662
C	-4.536607	0.520217	0.828790
C	-3.223812	-1.389350	0.172542
C	-5.543992	0.112019	-0.039390
H	-4.681790	1.439611	1.399568
C	-4.244530	-1.774411	-0.689678
H	-2.312744	-1.993469	0.209776
C	-5.430639	-1.042938	-0.819358
H	-6.451301	0.722811	-0.117038
H	-4.106941	-2.679982	-1.292845
C	-6.531819	-1.488091	-1.732967
H	-6.137843	-2.018455	-2.614493
H	-7.227933	-2.182447	-1.229373
H	-7.133218	-0.636622	-2.088675
H	-0.680916	5.810508	-1.675833
H	-2.282421	5.620789	-0.947316
H	-0.901819	6.149049	0.049848
H	5.660419	0.177773	2.560363
H	4.130007	0.166979	-4.083525
H	1.464470	-0.561537	3.251369
H	0.050183	-0.565579	-2.847747
C	5.397010	0.256615	-0.176713
C	5.094037	0.255020	-1.504452
H	6.425417	0.412989	0.161410
H	5.873349	0.410474	-2.255997

5f-s

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.446059

Total energy: -5331.837358310

C	1.020300	0.039904	-2.122302
C	-2.975219	0.040967	-0.155594
C	-4.301992	0.408725	-0.373961
C	-4.713787	0.824932	-1.641863
C	-3.748542	0.845205	-2.654476
C	-2.444830	0.471784	-2.360532
C	-2.472681	-0.451998	1.145438
C	-3.266309	-0.597589	2.283410
C	-2.712068	-1.109060	3.459004
C	-1.356994	-1.462273	3.434802
C	-0.629878	-1.285237	2.267457
H	-5.028851	0.371920	0.441774
H	-4.011589	1.155486	-3.669664
H	-1.673498	0.483030	-3.139507
H	-4.322539	-0.315887	2.265730
H	-0.872362	-1.872309	4.325397
H	0.432141	-1.556922	2.209087
N	-2.063453	0.091517	-1.142707
N	-1.174863	-0.786863	1.160546
Br	-0.370242	-2.785321	-1.189168
Ni	-0.136207	-0.418933	-0.561614
C	0.381917	1.304045	0.130410
C	-0.253221	2.501685	-0.210161
C	1.384866	1.361334	1.108774
C	0.097141	3.709239	0.401975
H	-1.038724	2.517376	-0.977282
C	1.737169	2.567121	1.717163
H	1.921983	0.451453	1.409381
H	-0.417884	4.632803	0.109005
H	2.529196	2.578590	2.476795
C	1.095959	3.766190	1.379200
C	-6.128895	1.204198	-1.914665
H	-6.187861	2.056262	-2.609189
H	-6.663502	0.365526	-2.393235
H	-6.669133	1.456954	-0.990737
C	-3.534373	-1.298383	4.687849
H	-4.465587	-0.714607	4.650622
H	-3.810797	-2.360587	4.803770
H	-2.972033	-1.017047	5.591655
C	1.454760	5.051993	2.059022
H	1.100878	-0.961410	-2.578906
H	0.402906	0.683558	-2.767454
N	2.298873	0.641566	-1.953041
C	2.480590	2.027693	-2.306779
H	3.391164	2.171694	-2.915576
H	1.627064	2.367791	-2.908168
H	2.564142	2.691408	-1.423999
C	3.261415	0.021885	-1.178079
C	4.455192	0.683942	-0.817710
C	3.071833	-1.284615	-0.675027

C	5.388873	0.073619	0.013301
H	4.653754	1.698997	-1.169082
C	4.020584	-1.871188	0.156512
H	2.163721	-1.848986	-0.911164
C	5.200153	-1.214581	0.526558
H	6.297289	0.627222	0.280430
H	3.829875	-2.882161	0.537684
C	6.222718	-1.868742	1.403622
H	5.762069	-2.593409	2.094298
H	6.975017	-2.424997	0.815152
H	6.775534	-1.129345	2.005478
H	0.951384	5.147863	3.037779
H	2.537380	5.121135	2.253915
H	1.159162	5.926655	1.458403

5f'-s

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.449107

Total energy: -5331.836808220

Ni	-0.876678	-0.360017	-0.302166
C	-2.696798	-0.743168	0.186016
C	-5.507149	-1.188909	0.336320
C	-3.265922	-1.410452	1.268187
C	-3.561278	-0.306784	-0.828894
C	-4.937163	-0.522491	-0.756356
C	-4.644304	-1.632493	1.342435
H	-2.640133	-1.786935	2.088820
H	-3.160795	0.214979	-1.710854
H	-5.586242	-0.169222	-1.567433
H	-5.060657	-2.167127	2.205361
N	-1.049358	1.771816	-0.220226
C	-0.899753	4.539901	0.164068
C	-2.089254	2.451365	0.265428
C	0.083573	2.433433	-0.504516
C	0.185176	3.813513	-0.330827
C	-2.060074	3.822500	0.474953
N	0.951314	0.273847	-1.066324
C	3.507368	1.264892	-1.653024
C	1.923115	-0.537533	-1.490207
C	1.210091	1.591845	-0.965959
C	2.469887	2.112267	-1.252710
C	3.202254	-0.089247	-1.792144
H	-2.983604	1.862705	0.501081
H	1.115041	4.336842	-0.566434
H	-2.938541	4.330945	0.881423
H	1.646092	-1.591683	-1.595066
H	2.661939	3.183810	-1.158476
H	3.963355	-0.804107	-2.118443
Br	-0.740868	-2.628304	-1.461455
C	4.887683	1.778909	-1.883160
H	4.893629	2.853583	-2.114880
H	5.494726	1.633346	-0.972520
H	5.391673	1.233337	-2.694498
C	-0.829669	6.019239	0.339720
H	-1.409589	6.347150	1.214908
H	0.207233	6.368583	0.445943
H	-1.260109	6.527282	-0.539791
C	-0.419639	-0.557490	1.622992
N	0.834030	-0.019224	1.947748
H	-1.208429	-0.054452	2.196552
H	-0.474671	-1.649786	1.749449
C	2.030094	-0.695723	1.703949
C	0.895977	1.323802	2.478571
C	3.272038	-0.077045	1.941400
C	2.046402	-2.012639	1.205074
H	-0.121895	1.714390	2.608611
H	1.399131	1.345169	3.460946
H	1.442419	2.015092	1.810339
C	4.463862	-0.743940	1.674831
H	3.322783	0.942067	2.329493
C	3.248129	-2.663212	0.955523
H	1.113983	-2.525387	0.956162
C	4.486038	-2.047442	1.170841
H	5.411149	-0.226461	1.866222
H	3.219607	-3.684640	0.558339
C	5.772111	-2.736737	0.833833
H	6.060512	-2.559093	-0.217781
H	6.603668	-2.375105	1.458522
H	5.695157	-3.827734	0.962709
C	-6.989056	-1.396749	0.425886
H	-7.243975	-2.202585	1.131390
H	-7.506798	-0.485664	0.773994
H	-7.423652	-1.650926	-0.554292

5g-s

Geometry with 56 atoms:

Thermal correction to Gibbs Free Energy: 0.384469

Total energy: -5251.286347320

Ni	-0.581233	-0.432552	-0.223775
N	-1.827510	-0.192260	1.457910
C	-3.041639	0.032934	1.140010
C	-1.788900	-0.351029	2.902984
C	-3.228526	-0.040421	3.339278
H	-1.473866	-1.381661	3.140362
H	-3.706994	-0.844084	3.915834
N	-2.429590	0.025427	-1.134991
C	-3.037369	0.119371	-2.454996
C	-3.372497	0.150436	-0.283214

C	-4.519600	0.393050	-2.156213
H	-2.563249	0.923934	-3.041139
H	-5.204651	-0.365647	-2.559892
O	-3.956633	0.109398	2.088651
O	-4.606324	0.346779	-0.705074
H	-1.047835	0.331887	3.348566
H	-3.323449	0.903981	3.896125
H	-2.871366	-0.824504	-3.001414
H	-4.858273	1.388090	-2.480008
C	0.110571	1.340501	0.014162
C	1.119306	1.518835	0.971875
C	1.604851	2.790285	1.280094
H	1.547368	0.651312	1.494372
C	0.086240	3.753665	-0.301885
C	1.094818	3.934113	0.649827
H	2.396536	2.901981	2.032013
H	-0.328266	4.631018	-0.814090
C	1.610853	5.296005	1.001521
H	1.307283	5.594467	2.020474
H	2.713091	5.330902	0.981582
H	1.235500	6.065094	0.308633
C	-0.397993	2.478920	-0.613773
Br	-0.930798	-2.855694	-0.061236
H	-1.183832	2.386987	-1.375591
C	0.574978	-0.506910	-1.844255
H	0.581388	-1.601213	-1.978764
H	-0.056643	-0.042448	-2.616764
N	1.878292	0.039554	-1.900340
C	2.091198	1.290137	-2.587488
H	2.264866	2.137153	-1.895974
H	2.960189	1.229767	-3.266395
H	1.210903	1.525770	-3.200061
C	2.879329	-0.445426	-1.074304
C	4.126505	0.205398	-0.971785
C	2.680979	-1.591759	-0.274061
C	5.114236	-0.272436	-0.115687
H	4.331397	1.106947	-1.553442
C	3.683857	-2.048135	0.574147
H	1.724378	-2.123664	-0.285657
C	4.924836	-1.408315	0.678143
H	6.067290	0.267116	-0.058337
H	3.487845	-2.935982	1.187848
C	6.001911	-1.928136	1.579243
H	5.583497	-2.397978	2.484170
H	6.619580	-2.696954	1.080409
H	6.687391	-1.126465	1.897677

5h-s

Geometry with 67 atoms:

Thermal correction to Gibbs Free Energy: 0.466346

Total energy: -5500.244669510

C	-3.298511	1.194643	2.712509
C	-2.435528	1.195364	1.613112
N	-2.269656	0.097024	0.872035
C	-2.935871	-1.029743	1.142869
C	-3.817240	-1.100906	2.224026
C	-3.989072	0.027805	3.017046
C	-1.676632	2.384624	1.164192
C	-2.673802	-2.159800	0.223423
C	-3.380220	-3.362991	0.284854
C	-3.080967	-4.368366	-0.627446
C	-2.090801	-4.144425	-1.577797
C	-1.434399	-2.917014	-1.568496
N	-0.874804	2.201421	0.105170
N	-1.710874	-1.956632	-0.691271
C	-0.217330	3.241814	-0.394385
C	-0.294631	4.521866	0.147366
C	-1.102864	4.715202	1.262644
C	-1.810006	3.634455	1.776005
Ni	-0.779064	0.023286	-0.559749
H	-3.432066	2.087523	3.325123
H	-4.357838	-2.021014	2.451414
H	-4.666018	-0.001337	3.873755
H	-4.162155	-3.514802	1.031069
H	-3.622789	-5.316711	-0.597039
H	-1.826616	-4.902305	-2.317808
H	-0.651770	-2.700844	-2.304369
H	0.406409	3.046023	-1.272347
H	0.269652	5.342642	-0.299833
H	-1.191442	5.700703	1.726286
H	-2.464353	3.768989	2.639267
C	0.571776	-0.376049	0.795750
C	1.518993	0.584091	1.171256
C	0.600839	-1.593474	1.484651
C	2.444472	0.346431	2.185433
H	1.573086	1.541428	0.638460
C	1.529855	-1.837666	2.501159
H	-0.102902	-2.396731	1.229785
C	2.474672	-0.875105	2.867228
H	3.181598	1.119976	2.438420
H	1.524199	-2.806364	3.016793
C	3.516678	-1.149936	3.908880
H	4.490707	-1.391745	3.446145
H	3.686168	-0.275933	4.558550
H	3.241536	-2.002934	4.548431
C	0.718446	-0.474581	-1.804787
H	0.105047	-0.478456	-2.719995
H	0.974419	-1.504923	-1.529570

N	1.871965	0.315533	-1.996573
C	3.111662	0.010702	-1.445188
C	3.364902	-1.211923	-0.788120
C	4.183831	0.921430	-1.526396
C	4.599775	-1.478176	-0.217565
H	2.577445	-1.960277	-0.686776
C	5.416266	0.636620	-0.941298
H	4.062917	1.878506	-2.037876
C	5.657249	-0.559692	-0.262900
H	4.744700	-2.436795	0.296188
H	6.218790	1.379661	-1.018825
C	6.969191	-0.849927	0.400043
H	6.904386	-0.745451	1.497684
H	7.306424	-1.880919	0.202938
H	7.758495	-0.164088	0.055518
C	1.747083	1.489021	-2.826609
H	0.703003	1.583666	-3.158746
H	2.019780	2.417175	-2.291409
H	2.396715	1.430610	-3.719543
Br	-2.288488	0.784730	-2.479514

TS5a,1a'

Geometry with 58 atoms:

Thermal correction to Gibbs Free Energy: 0.398696

Total energy: -5253.221580630

C	-0.821820	-0.253626	1.629872
C	3.359179	-0.543206	0.528977
C	4.593788	-0.688808	1.163478
C	4.636790	-1.212008	2.450647
C	3.448466	-1.584985	3.070347
C	2.258332	-1.404295	2.374466
C	3.214890	-0.032684	-0.852160
C	4.276472	0.464955	-1.611045
C	4.026786	0.906101	-2.906147
C	2.732016	0.837792	-3.413438
C	1.730355	0.332309	-2.591502
H	5.517261	-0.407345	0.654358
H	3.435971	-2.010468	4.075392
H	1.300674	-1.688554	2.825070
H	5.286075	0.515987	-1.199286
H	2.497827	1.171530	-4.426160
H	0.690755	0.258021	-2.934796
N	2.212470	-0.887894	1.146316
N	1.971505	-0.086424	-1.352958
Br	-0.041353	-2.808816	-0.936682
Ni	0.499169	-0.584570	0.027390
C	0.008849	1.213163	0.404087
C	0.818347	2.116154	1.101369
C	-0.885225	1.725426	-0.549422
C	0.764317	3.481547	0.825047
H	1.505757	1.753108	1.876635
C	-0.925694	3.090222	-0.828417
H	-1.564659	1.047161	-1.083323
H	1.410061	4.169699	1.383543
H	-1.622073	3.465186	-1.587911
C	-0.099451	3.995700	-0.150270
C	-0.129312	5.459718	-0.468169
H	-0.907896	-1.354695	1.553272
H	-0.193872	-0.018619	2.500757
N	-2.101296	0.332195	1.797148
C	-2.185024	1.557950	2.555223
H	-3.055032	1.543228	3.232646
H	-1.284391	1.667696	3.173563
H	-2.266563	2.455510	1.910845
C	-3.186266	-0.036099	1.009343
C	-4.369561	0.729376	0.993900
C	-3.150989	-1.181896	0.189687
C	-5.458704	0.347762	0.214480
H	-4.449887	1.642361	1.587018
C	-4.247961	-1.538604	-0.584790
H	-2.250547	-1.796891	0.123528
C	-5.433081	-0.793436	-0.591327
H	-6.359751	0.972308	0.229483
H	-4.171147	-2.432321	-1.216367
C	-6.616909	-1.210250	-1.409877
H	-6.310173	-1.657956	-2.368794
H	-7.229555	-1.967448	-0.888965
H	-7.278955	-0.357884	-1.628751
H	0.569729	5.710033	-1.285727
H	-1.129737	5.784317	-0.794617
H	0.162867	6.070388	0.400235
H	4.842682	1.302100	-3.515594
H	5.594899	-1.334701	2.961197

TS5b,1b'

Geometry with 82 atoms:

Thermal correction to Gibbs Free Energy: 0.608399

Total energy: -5567.605717340

C	-1.876787	-1.338825	1.081881
C	2.174155	-0.882427	-0.169505
C	3.424754	-1.419219	0.114285
C	3.544848	-2.720347	0.619419
C	2.355663	-3.430290	0.805095
C	1.139999	-2.828079	0.499003
C	1.979838	0.476669	-0.720315
C	2.945376	1.475169	-0.651853
C	2.671299	2.758253	-1.143686
C	1.416944	2.951583	-1.730062

C	0.505491	1.900964	-1.761708
H	4.317843	-0.819856	-0.081256
H	2.352008	-4.453184	1.184301
H	0.200719	-3.377096	0.634541
H	3.904327	1.262537	-0.171794
H	1.123599	3.914972	-2.149877
H	-0.494834	2.039164	-2.191216
N	1.043122	-1.584905	0.035980
N	0.770350	0.700962	-1.259565
Br	-1.399263	-1.799957	-2.544372
Ni	-0.695778	-0.609258	-0.488875
C	-1.010666	0.577782	0.964488
C	-0.062690	0.832617	1.960735
C	-1.925578	1.592179	0.647215
C	0.013841	2.085178	2.568259
H	0.642582	0.047173	2.262721
C	-1.841306	2.844194	1.254482
H	-2.712765	1.408624	-0.096244
H	0.776237	2.266390	3.335494
H	-2.553621	3.629155	0.973777
C	-0.861874	3.120714	2.216879
C	-0.743821	4.480669	2.834573
H	-2.058791	-2.148942	0.350119
H	-1.170775	-1.708590	1.838771
N	-3.088903	-0.953913	1.704597
C	-3.027730	-0.479438	3.066730
H	-3.841109	-0.912223	3.672876
H	-2.076293	-0.788220	3.519119
H	-3.096966	0.624056	3.138320
C	-4.246085	-0.719403	0.970951
C	-5.372522	-0.112441	1.562114
C	-4.343071	-1.066463	-0.391993
C	-6.534249	0.109387	0.827483
H	-5.351223	0.203247	2.606902
C	-5.511800	-0.829763	-1.105468
H	-3.492214	-1.500795	-0.922920
C	-6.640819	-0.244627	-0.520088
H	-7.387168	0.586188	1.324841
H	-5.539342	-1.106234	-2.166653
C	-7.902438	-0.024457	-1.297929
H	-7.691947	0.241379	-2.346277
H	-8.532948	-0.931057	-1.321901
H	-8.514066	0.779447	-0.859324
H	-0.083393	5.136432	2.239582
H	-1.720513	4.985427	2.897587
H	-0.316353	4.431936	3.848166
C	3.701374	3.868114	-0.990381
C	3.230007	5.174453	-1.620033
H	4.004805	5.947107	-1.489935
H	3.046931	5.067709	-2.702295
H	2.307351	5.550727	-1.147573
C	3.935386	4.102544	0.506391
H	4.329202	3.205769	1.011435
H	4.665747	4.916147	0.651201
H	2.997791	4.391490	1.011294
C	5.010776	3.444532	-1.662464
H	4.861199	3.259165	-2.739350
H	5.762657	4.244239	-1.556445
H	5.434977	2.531010	-1.216039
C	4.920024	-3.295089	0.927683
C	4.833953	-4.717353	1.470644
H	4.374036	-5.408953	0.745299
H	5.847862	-5.091549	1.685281
H	4.258311	-4.765952	2.409949
C	5.752260	-3.310522	-0.358653
H	5.272929	-3.932475	-1.133080
H	5.897006	-2.300574	-0.774637
H	6.750643	-3.731533	-0.153500
C	5.601740	-2.410109	1.976429
H	5.739222	-1.375476	1.623371
H	5.013622	-2.376424	2.908861
H	6.598982	-2.814543	2.217325

TS5c,1c'

Geometry with 66 atoms:

Thermal correction to Gibbs Free Energy: 0.457927

Total energy: -5482.247991520

C	-1.360953	-1.425634	0.931114
C	2.781345	-0.770140	-0.049808
C	4.016846	-1.306058	0.276071
C	4.095513	-2.620485	0.758317
C	2.909048	-3.352872	0.886384
C	1.718375	-2.728599	0.539737
C	2.620067	0.598530	-0.593780
C	3.661762	1.509614	-0.682914
C	3.414035	2.783140	-1.215524
C	2.116366	3.087481	-1.647083
C	1.140721	2.107569	-1.513996
H	4.943257	-0.740893	0.156922
H	2.890880	-4.383261	1.243158
H	0.774860	-3.279289	0.629075
H	4.673084	1.276992	-0.343373
H	1.854051	4.056477	-2.073611
H	0.109734	2.305292	-1.833977
N	1.638492	-1.476008	0.094887
N	1.376578	0.903592	-1.005935
Br	-0.722439	-1.195215	-2.718739
Ni	-0.088357	-0.459140	-0.427753

C	-0.554640	0.489937	1.148328
C	0.282304	0.613790	2.262521
C	-1.471921	1.520048	0.891715
C	0.233165	1.751014	3.067173
H	0.989851	-0.188375	2.510275
C	-1.508391	2.659198	1.694217
H	-2.173083	1.432917	0.050700
H	0.901721	1.827367	3.933071
H	-2.223292	3.458401	1.464735
C	-0.653739	2.800439	2.794964
C	-0.676338	4.036882	3.641307
H	-1.456396	-2.124563	0.077478
H	-0.706598	-1.890860	1.681820
N	-2.631254	-1.167605	1.506627
C	-2.681560	-0.884240	2.921168
H	-3.545981	-1.382672	3.390493
H	-1.773660	-1.269493	3.403955
H	-2.749653	0.199760	3.140793
C	-3.739281	-0.852004	0.728205
C	-4.902471	-0.300864	1.302587
C	-3.747933	-1.061244	-0.665198
C	-6.012276	0.004666	0.518713
H	-4.949292	-0.091388	2.373004
C	-4.864354	-0.741676	-1.427736
H	-2.865979	-1.449455	-1.179366
C	-6.028454	-0.207410	-0.862234
H	-6.895648	0.435867	1.004476
H	-4.820312	-0.909036	-2.511145
C	-7.233628	0.104980	-1.696053
H	-6.951446	0.475955	-2.694435
H	-7.864062	-0.787644	-1.856810
H	-7.871118	0.865401	-1.218413
H	0.018463	4.803653	3.255142
H	-1.676941	4.496241	3.663582
H	-0.373152	3.825332	4.678582
O	4.448718	3.618787	-1.268734
O	5.308383	-3.077565	1.052825
C	4.257806	4.918437	-1.788071
H	5.227019	5.427445	-1.731461
H	3.929897	4.885742	-2.840492
H	3.519683	5.482753	-1.193934
C	5.449360	-4.398974	1.534089
H	5.091284	-5.134098	0.794462
H	6.519506	-4.559104	1.708856
H	4.904520	-4.539804	2.482309

TS5d,1d'

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.453497

Total energy: -5331.835734960

C	0.727737	-0.405659	-1.923616
C	-3.137012	-0.154287	0.436789
C	-4.503277	0.080930	0.298281
C	-5.158042	-0.427513	-0.818168
C	-4.438378	-1.162972	-1.748903
C	-3.065870	-1.358650	-1.558840
C	-2.365409	0.313281	1.611233
C	-2.874492	1.213231	2.546791
C	-2.078414	1.558612	3.633975
C	-0.819296	0.987221	3.767164
C	-0.359608	0.106324	2.783030
H	-5.055345	0.636350	1.058035
H	-4.924596	-1.589881	-2.629421
H	-3.869337	1.646423	2.430444
H	-0.181196	1.221017	4.622972
N	-2.443739	-0.846826	-0.487904
N	-1.126247	-0.192324	1.725761
Br	0.112130	-3.208052	0.273009
Ni	-0.400650	-0.771133	-0.150705
C	-0.205847	1.047153	-0.761732
C	-1.197576	1.713433	-1.493689
C	0.645877	1.835082	0.029892
C	-1.381398	3.090559	-1.377185
H	-1.857075	1.152277	-2.168029
C	0.451204	3.208241	0.154657
H	1.480469	1.372952	0.569952
H	-2.173918	3.576502	-1.958471
H	1.117770	3.787403	0.804771
C	-0.575674	3.865288	-0.535828
C	-0.803358	5.336422	-0.369832
H	0.914781	-1.487927	-1.801366
H	0.062083	-0.273249	-2.785128
N	1.944810	0.287827	-2.144602
C	1.916950	1.444627	-3.008602
H	2.803336	1.466730	-3.663889
H	1.029235	1.396104	-3.653068
H	1.879924	2.400292	-2.449001
C	3.025038	0.121973	-1.285622
C	4.108919	1.023810	-1.295205
C	3.075412	-0.934520	-0.353994
C	5.177565	0.867407	-0.418401
H	4.119392	1.873246	-1.980972
C	4.151884	-1.065798	0.517202
H	2.263446	-1.663699	-0.282178
C	5.231378	-0.176576	0.510760
H	5.996363	1.595753	-0.452220
H	4.142080	-1.894857	1.235813
C	6.396338	-0.347292	1.437341

H	6.096770	-0.834686	2.378548
H	7.186773	-0.975999	0.990221
H	6.861782	0.619285	1.686945
H	-1.434249	5.549401	0.511304
H	0.142773	5.880331	-0.220648
H	-1.314659	5.770165	-1.243056
H	-6.229438	-0.259240	-0.951795
H	-2.446569	2.267177	4.380069
C	0.990315	-0.522594	2.854432
H	0.921591	-1.603889	2.652394
H	1.657203	-0.109804	2.076366
H	1.463973	-0.355103	3.831173
C	-2.249723	-2.112777	-2.552618
H	-1.726974	-1.417862	-3.232382
H	-1.485709	-2.723022	-2.044981
H	-2.882253	-2.759117	-3.176658

TS5e,1e'

Geometry with 60 atoms:

Thermal correction to Gibbs Free Energy: 0.412385

Total energy: -5329.422619840

C	-1.092647	-0.138934	1.655526
C	3.065155	-0.499866	0.619097
C	4.336197	-0.488437	1.234044
C	4.394508	-0.824104	2.602218
C	3.233071	-1.150982	3.269807
C	2.015337	-1.124583	2.570607
C	2.954073	-0.189056	-0.780500
C	4.108893	0.141344	-1.522465
C	3.930136	0.432876	-2.890780
C	2.665215	0.378126	-3.439387
C	1.580716	0.031991	-2.615186
H	3.242126	-1.424343	4.326487
H	2.496067	0.595855	-4.495752
N	1.928639	-0.799234	1.290762
N	1.725932	-0.239822	-1.332422
Br	-0.369380	-2.836983	-0.793619
Ni	0.229495	-0.596045	0.089983
C	-0.244656	1.230070	0.322193
C	0.559824	2.182796	0.955618
C	-1.131091	1.667523	-0.673934
C	0.505694	3.524159	0.578797
H	1.242568	1.880526	1.760501
C	-1.171985	3.007826	-1.053192
H	-1.804249	0.948638	-1.160586
H	1.146642	4.252970	1.089137
H	-1.862921	3.324318	-1.843650
C	-0.352536	3.962845	-0.436978
C	-0.383480	5.399551	-0.861636
H	-1.180143	-1.242780	1.665024
H	-0.467389	0.163050	2.506920
N	-2.368934	0.465389	1.770394
C	-2.447359	1.745703	2.432782
H	-3.335183	1.795078	3.084734
H	-1.561818	1.884736	3.066971
H	-2.495017	2.595242	1.723219
C	-3.452735	0.049351	1.003891
C	-4.612263	0.842144	0.889309
C	-3.439171	-1.174457	0.306286
C	-5.698620	0.415402	0.129515
H	-4.674742	1.812798	1.385092
C	-4.532050	-1.576013	-0.451562
H	-2.557369	-1.818562	0.322294
C	-5.693170	-0.800888	-0.557948
H	-6.580221	1.063856	0.062992
H	-4.471413	-2.530927	-0.988307
C	-6.873823	-1.263508	-1.356172
H	-6.563098	-1.815157	-2.257927
H	-7.519728	-1.945550	-0.775104
H	-7.504375	-0.418669	-1.674502
H	0.324136	5.592192	-1.687386
H	-1.381145	5.695251	-1.222148
H	-0.103255	6.073326	-0.037066
H	5.360719	-0.825666	3.115243
H	4.798812	0.696312	-3.501320
H	1.080658	-1.377193	3.084246
H	0.561392	-0.027658	-3.017244
C	5.491131	-0.145637	0.456685
C	5.382336	0.159575	-0.865910
H	6.465031	-0.137271	0.954395
H	6.266695	0.420065	-1.454600

TS5f,1f'

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.445774

Total energy: -5331.825064170

C	1.151854	-0.740124	-1.471204
C	-3.053131	-0.678611	-0.411296
C	-4.279278	-0.996672	-0.993769
C	-4.332847	-1.848001	-2.099017
C	-3.118444	-2.353788	-2.575376
C	-1.936645	-1.989295	-1.947900
C	-2.929791	0.186425	0.783803
C	-4.008597	0.843015	1.378054
C	-3.805324	1.625946	2.516376
C	-2.499899	1.711475	3.016200
C	-1.479167	1.031331	2.368714
H	-5.207461	-0.589787	-0.584165

H	-3.094211	-3.030324	-3.434424
H	-0.976244	-2.377508	-2.306174
H	-5.014537	0.757816	0.957901
H	-2.282993	2.310285	3.905622
H	-0.445171	1.074989	2.733821
N	-1.896097	-1.164724	-0.899467
N	-1.689714	0.293621	1.281334
Br	0.401043	-2.299548	1.779756
Ni	-0.200137	-0.576857	0.132224
C	0.322160	1.027355	-0.742372
C	-0.459843	1.692341	-1.695097
C	1.206844	1.795005	0.032449
C	-0.390291	3.077488	-1.837334
H	-1.138383	1.120759	-2.342071
C	1.264112	3.181331	-0.106811
H	1.863298	1.301763	0.762612
H	-1.016812	3.574158	-2.588495
H	1.951631	3.759154	0.522965
C	0.464028	3.852212	-1.041247
C	-5.628147	-2.227238	-2.730405
H	-5.554569	-2.213835	-3.829023
H	-5.906840	-3.256066	-2.444516
H	-6.445500	-1.560847	-2.419138
C	-4.933054	2.331498	3.189398
H	-5.832174	2.362191	2.557121
H	-5.200425	1.819477	4.129678
H	-4.652858	3.361659	3.460016
C	0.507809	5.343322	-1.173532
H	1.235502	-1.768064	-1.068689
H	0.531639	-0.776558	-2.377456
N	2.434743	-0.230801	-1.803521
C	2.531194	0.686940	-2.913093
H	3.380196	0.427916	-3.569000
H	1.617276	0.628897	-3.519084
H	2.663619	1.739480	-2.592994
C	3.525954	-0.360060	-0.955983
C	4.724260	0.343933	-1.196239
C	3.486017	-1.190291	0.183480
C	5.821211	0.201556	-0.348924
H	4.811337	1.021238	-2.048421
C	4.591159	-1.310830	1.016321
H	2.573419	-1.726873	0.457501
C	5.790715	-0.628696	0.774434
H	6.733575	0.768094	-0.571335
H	4.510372	-1.959083	1.898217
C	6.978950	-0.795415	1.670396
H	6.685884	-0.839165	2.732461
H	7.526053	-1.731607	1.457282
H	7.697430	0.030930	1.550564
H	-0.243932	5.830038	-0.526097
H	1.489399	5.749725	-0.882130
H	0.295454	5.667742	-2.204874

TS5f',1f'

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.451531

Total energy: -5331.809786700

Ni	-0.815872	-0.067576	-0.275171
C	-2.563895	-0.158348	0.622767
C	-5.370318	-0.336973	0.104071
C	-3.322634	-1.269579	1.026726
C	-3.256268	0.869415	-0.038045
C	-4.623835	0.767421	-0.306817
C	-4.684280	-1.357368	0.778724
H	-2.833497	-2.113723	1.528453
H	-2.741413	1.753496	-0.418026
H	-5.118434	1.578576	-0.853963
H	-5.232796	-2.249338	1.103488
N	-0.196483	2.047182	-0.129738
C	0.915109	4.635921	-0.082319
C	-0.858533	3.084877	0.387902
C	1.049665	2.268517	-0.586763
C	1.618601	3.543311	-0.590323
C	-0.355062	4.376600	0.438711
N	1.091247	-0.058146	-1.137769
C	3.851579	-0.060157	-1.636420
C	1.722231	-1.172203	-1.517195
C	1.802308	1.075293	-1.033254
C	3.176029	1.107604	-1.278353
C	3.083928	-1.219068	-1.775379
H	-1.848142	2.880582	0.810111
H	2.622917	3.696868	-0.992045
H	-0.953284	5.175536	0.884634
H	1.089493	-2.060812	-1.614911
H	3.741498	2.035030	-1.160438
H	3.548869	-2.165840	-2.066419
Br	-1.520763	-2.048472	-1.749676
C	5.331905	-0.089687	-1.816256
H	5.757875	0.919361	-1.908716
H	5.804474	-0.576040	-0.944836
H	5.617181	-0.679206	-2.700949
C	1.488211	6.012311	-0.102690
H	1.153320	6.599511	0.764952
H	2.587342	5.995095	-0.121131
H	1.153030	6.550853	-1.005215
C	-1.134508	-0.085084	1.913353
N	0.262375	0.167193	2.110642
H	-1.687675	0.676745	2.478875

H	-1.385035	-1.069991	2.331873
C	1.203751	-0.838394	1.902917
C	0.690097	1.404113	2.720229
C	2.575418	-0.602187	2.118590
C	0.831054	-2.120520	1.457754
H	-0.181947	2.042763	2.909954
H	1.189306	1.221089	3.689137
H	1.394469	1.975245	2.086746
C	3.517004	-1.596310	1.876457
H	2.923620	0.375140	2.459420
C	1.789129	-3.103551	1.231743
H	-0.212809	-2.349559	1.229637
C	3.153352	-2.868201	1.422121
H	4.577405	-1.369013	2.040332
H	1.458553	-4.084140	0.869274
C	4.189750	-3.902000	1.104906
H	4.706593	-3.673759	0.154919
H	4.969422	-3.952656	1.882301
H	3.746871	-4.904357	1.001027
C	-6.844011	-0.427907	-0.142207
H	-7.420756	-0.172625	0.763961
H	-7.166026	0.261649	-0.937300
H	-7.143911	-1.448489	-0.429346

TS5g,1g'

Geometry with 56 atoms:

Thermal correction to Gibbs Free Energy: 0.385091

Total energy: -5251.275130000

Ni	0.556098	-0.523555	-0.025905
N	2.196655	0.061529	-1.339436
C	3.309163	-0.044662	-0.724897
C	2.456996	0.880173	-2.516813
C	3.985306	1.047762	-2.519491
H	2.076016	0.390564	-3.425721
H	4.485751	0.477351	-3.316316
N	2.218383	-0.927484	1.173712
C	2.531518	-1.677486	2.384047
C	3.329739	-0.706410	0.583126
C	4.068259	-1.681396	2.422890
H	2.081721	-1.198980	3.268050
H	4.515232	-2.682294	2.486290
O	4.401648	0.488345	-1.247715
O	4.454318	-1.097771	1.151490
H	1.912750	1.836108	-2.409969
H	4.326387	2.090842	-2.559996
H	2.093739	-2.687630	2.300796
H	4.488200	-1.050937	3.220468
C	0.056051	1.272614	0.329459
C	-0.841807	1.763396	-0.630471
C	-0.883010	3.123325	-0.936607
H	-1.519485	1.074276	-1.151838
C	0.823349	3.545459	0.694417
C	-0.055370	4.041420	-0.278284
H	-1.577268	3.482987	-1.705269
H	1.482511	4.243438	1.224335
C	-0.131174	5.507719	-0.576887
H	-0.456807	5.694457	-1.612055
H	-0.853941	6.018884	0.083169
H	0.841245	6.002721	-0.427752
C	0.877324	2.186546	0.997851
Br	0.190034	-2.819894	-0.895184
H	1.578242	1.832074	1.764764
C	-0.738371	-0.188089	1.584927
H	-0.781452	-1.293195	1.533904
H	-0.107032	0.086205	2.440837
N	-2.033661	0.357582	1.741894
C	-2.158446	1.595756	2.474036
H	-2.285211	2.473277	1.809450
H	-3.017887	1.562460	3.164047
H	-1.254861	1.756194	3.076566
C	-3.102007	-0.060631	0.955616
C	-4.321169	0.646249	0.949147
C	-3.012132	-1.197673	0.127762
C	-5.393478	0.215981	0.172372
H	-4.444160	1.549772	1.549399
C	-4.094499	-1.603729	-0.643655
H	-2.081289	-1.765282	0.051765
C	-5.315096	-0.918519	-0.639675
H	-6.324233	0.795012	0.194747
H	-3.976780	-2.488271	-1.281643
C	-6.481558	-1.389011	-1.453947
H	-7.172582	-0.563845	-1.687142
H	-6.156825	-1.840519	-2.404986
H	-7.068821	-2.158590	-0.922058

TS5h,1h'

Geometry with 67 atoms:

Thermal correction to Gibbs Free Energy: 0.465839

Total energy: -5500.235306260

C	-2.458199	1.179348	3.173254
C	-2.054410	1.239848	1.837626
N	-2.198440	0.186642	1.029972
C	-2.733002	-0.956090	1.465682
C	-3.175173	-1.087696	2.783500
C	-3.025501	-0.002162	3.641481
C	-1.441391	2.424615	1.196335
C	-2.763036	-2.041912	0.461298
C	-3.536752	-3.193255	0.612470

C	-3.502319	-4.161640	-0.384915
C	-2.701477	-3.951618	-1.503012
C	-1.963761	-2.773348	-1.575939
N	-0.956315	2.224498	-0.040284
N	-1.986227	-1.847604	-0.620164
C	-0.459175	3.255926	-0.715805
C	-0.370649	4.537978	-0.179759
C	-0.836101	4.745084	1.115027
C	-1.391203	3.677152	1.811201
Ni	-0.954644	0.075991	-0.618553
H	-2.324098	2.031107	3.842795
H	-3.602912	-2.025247	3.144134
H	-3.342985	-0.080646	4.683751
H	-4.171644	-3.324232	1.491380
H	-4.102675	-5.069858	-0.291157
H	-2.646692	-4.683462	-2.311312
H	-1.328203	-2.564836	-2.444566
H	-0.116893	3.046405	-1.735561
H	0.054906	5.352007	-0.770046
H	-0.782589	5.734190	1.576516
H	-1.794338	3.821771	2.815699
C	0.590489	-0.353764	0.494014
C	1.459727	0.672262	0.890516
C	0.567995	-1.505132	1.294773
C	2.211614	0.583483	2.059814
H	1.566112	1.569455	0.269712
C	1.319141	-1.595903	2.465362
H	-0.049572	-2.364147	1.002534
C	2.155855	-0.551558	2.876409
H	2.869610	1.415203	2.340857
H	1.261896	-2.508091	3.071877
C	3.006618	-0.666966	4.104137
H	4.021324	-1.028285	3.857530
H	3.130682	0.305458	4.606840
H	2.580977	-1.376981	4.830349
C	0.732659	-0.711217	-1.585714
H	0.009439	-0.685215	-2.420142
H	0.932469	-1.762607	-1.349256
N	1.895989	-0.006459	-1.966287
C	3.152362	-0.295099	-1.442157
C	3.425211	-1.511292	-0.781879
C	4.215457	0.620222	-1.557984
C	4.677144	-1.769356	-0.243647
H	2.643267	-2.264019	-0.663208
C	5.466317	0.342036	-1.009826
H	4.069966	1.577539	-2.062725
C	5.730064	-0.848257	-0.330062
H	4.842787	-2.724349	0.269633
H	6.263126	1.087989	-1.112836
C	7.063122	-1.132895	0.291867
H	7.019557	-1.076527	1.393831
H	7.420864	-2.146053	0.044211
H	7.827514	-0.414277	-0.041336
C	1.721500	1.199897	-2.738214
H	0.694856	1.230796	-3.133085
H	1.886044	2.118191	-2.139891
H	2.421526	1.234595	-3.590640
Br	-2.237375	0.780991	-2.795262

CP-2f-s

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.449418

Total energy: -5331.889379320

C	1.354284	-0.951963	-1.044008
C	-2.935761	-1.143867	-0.219223
C	-3.826289	-1.955665	-0.920941
C	-3.501055	-3.289321	-1.179429
C	-2.270390	-3.754065	-0.700266
C	-1.434625	-2.886376	-0.012122
C	-3.214624	0.265399	0.134012
C	-4.390121	0.926249	-0.215494
C	-4.601124	2.246950	0.191075
C	-3.604545	2.841999	0.970696
C	-2.451126	2.127437	1.264170
H	-4.783697	-1.558804	-1.269766
H	-1.965694	-4.791848	-0.864719
H	-0.469540	-3.221593	0.387117
H	-5.156567	0.416750	-0.805870
H	-3.722208	3.864175	1.342560
H	-1.653008	2.578281	1.863791
N	-1.749332	-1.609769	0.212666
N	-2.246494	0.877056	0.846274
Br	0.809725	-1.285181	2.672888
Ni	-0.516919	-0.171380	0.978696
C	0.629035	0.351016	-0.777137
C	-0.262812	0.856796	-1.758077
C	1.047775	1.244121	0.244690
C	-0.699745	2.166873	-1.733142
H	-0.610346	0.180744	-2.549675
C	0.613832	2.585058	0.233234
H	1.840013	0.950551	0.940188
H	-1.403694	2.521750	-2.495716
H	0.973530	3.266672	1.013504
C	-0.258231	3.064777	-0.736187
C	-4.437739	-4.192327	-1.907588
H	-3.895851	-4.865126	-2.590212
H	-4.984033	-4.834672	-1.195272
H	-5.185312	-3.627039	-2.483280

C	-5.830441	2.992251	-0.202292
H	-6.668717	2.312023	-0.414006
H	-6.135853	3.706323	0.577456
H	-5.644386	3.577823	-1.119526
C	-0.710155	4.491850	-0.744932
H	1.587219	-1.465288	-0.099786
H	0.685102	-1.626604	-1.606525
N	2.571561	-0.783119	-1.824202
C	2.392256	-0.507606	-3.226731
H	3.223340	-0.920719	-3.822383
H	1.469352	-0.993276	-3.576589
H	2.317230	0.574723	-3.463321
C	3.757156	-0.402649	-1.210216
C	4.801159	0.197199	-1.943901
C	3.992435	-0.614056	0.168943
C	6.010461	0.536257	-1.338034
H	4.676490	0.412472	-3.007375
C	5.203239	-0.264581	0.751137
H	3.223023	-1.055002	0.810348
C	6.248550	0.315973	0.019259
H	6.792627	1.000287	-1.950991
H	5.339680	-0.447808	1.824159
C	7.549747	0.670179	0.670464
H	7.398015	1.232782	1.607196
H	8.133240	-0.228924	0.937821
H	8.181034	1.283278	0.008285
H	-1.740268	4.588692	-1.125966
H	-0.671192	4.938318	0.261926
H	-0.073206	5.114388	-1.398881

6

Geometry with 36 atoms:

Thermal correction to Gibbs Free Energy: 0.25945

Total energy: -675.616390420

N	-0.611001	1.808173	0.150135
C	-1.563140	0.807142	0.117843
C	-1.489203	-0.321176	0.966241
C	-2.657692	0.867431	-0.770006
C	-2.463038	-1.311014	0.926827
H	-0.656516	-0.435219	1.665046
C	-3.620272	-0.139309	-0.792725
H	-2.769495	1.713940	-1.451421
C	-3.553336	-1.252481	0.049044
H	-2.368466	-2.168619	1.604115
H	-4.456922	-0.050238	-1.496153
C	-4.576139	-2.345915	0.004945
H	-4.182516	-3.257887	-0.478735
H	-4.899981	-2.643977	1.016309
H	-5.471426	-2.040625	-0.559196
C	0.549236	1.688712	0.997859
H	0.985791	2.696061	1.115324
H	0.250538	1.396708	2.021937
C	-0.661583	2.870391	-0.823410
H	-1.571572	3.490247	-0.718689
H	0.205425	3.531867	-0.689805
C	1.621267	0.744260	0.504205
C	2.651487	0.352294	1.368381
C	1.636295	0.257649	-0.803348
C	3.666658	-0.491262	0.933065
H	2.651491	0.718443	2.402191
C	2.655462	-0.591388	-1.237188
H	0.835466	0.538535	-1.496410
C	3.688829	-0.981130	-0.381172
H	4.463722	-0.785951	1.625977
H	2.645739	-0.962805	-2.268293
C	4.783193	-1.897075	-0.833142
H	-0.637332	2.495825	-1.865813
H	4.687085	-2.152496	-1.899431
H	5.777232	-1.443228	-0.681749
H	4.780592	-2.840565	-0.260667

Br-

Geometry with 1 atoms:

Thermal correction to Gibbs Free Energy: -0.016176

Total energy: -2574.136168480

Br	0.000000	0.000000	0.000000

MECP at 3

Geometry with 42 atoms:

Thermal correction to Gibbs Free Energy: 0.271261

Total energy: -4927.061797870

Ni	0.333156	-0.684167	-0.450258
N	-0.387822	1.183376	-0.664841
C	2.080982	-0.125270	0.202752
N	-1.612827	-0.921982	0.247196
Br	0.718606	-2.900737	-1.160112
C	0.328934	2.201680	-1.158394
C	-0.184109	3.490586	-1.266522
C	-1.491079	3.757350	-0.829169
C	-2.222346	2.683097	-0.307462
C	-1.653562	1.406409	-0.244201
C	-2.351544	0.205749	0.275601
C	-3.664900	0.202656	0.761346
C	-4.231295	-0.985038	1.239454
C	-3.435474	-2.141965	1.194202
C	-2.140424	-2.069827	0.689384
C	3.302853	-0.641516	-0.268161
C	4.526459	-0.198501	0.242938

C	4.587147	0.765975	1.263151
C	3.375001	1.275565	1.747636
C	2.150960	0.842647	1.219976
C	-5.630768	-1.027885	1.791315
C	-2.087390	5.134847	-0.936512
C	5.917703	1.227868	1.808739
H	1.352464	1.958706	-1.450304
H	0.440976	4.285675	-1.678366
H	-3.238896	2.847820	0.052223
H	-4.252890	1.121371	0.769965
H	-3.824623	-3.100408	1.545370
H	-1.487770	-2.943623	0.605539
H	3.292402	-1.413245	-1.041864
H	5.458556	-0.619164	-0.150681
H	3.386935	2.022088	2.549395
H	1.229117	1.277494	1.623317
H	-6.207691	-1.850562	1.340073
H	-5.610692	-1.208044	2.879346
H	-6.172123	-0.087502	1.613524
H	-2.489769	5.300443	-1.950915
H	-2.913763	5.277942	-0.224663
H	-1.331291	5.913488	-0.755022
H	5.793578	1.953323	2.627622
H	6.508332	0.381039	2.197971
H	6.529228	1.709278	1.025684

[anethole]˙+

Geometry with 23 atoms:

Thermal correction to Gibbs Free Energy: 0.155404

Total energy: -463.135857675

H	-0.321412	-2.325759	0.000224
C	0.049825	-1.296536	0.000183
C	0.939968	1.358211	0.000192
C	-0.900478	-0.229854	0.000217
C	1.400602	-1.063990	0.000066
C	1.869865	0.276519	0.000056
C	-0.401176	1.111081	0.000260
H	2.101065	-1.901315	0.000005
H	-1.095897	1.954282	0.000414
H	1.345263	2.372899	0.000254
O	3.130127	0.614868	-0.000057
C	4.170179	-0.358712	-0.000342
H	4.112903	-0.984929	0.903596
H	5.112131	0.199636	-0.000580
H	4.112433	-0.984917	-0.904257
H	-2.533604	-1.622833	0.000525
C	-2.283577	-0.553865	0.000201
C	-3.326212	0.341653	-0.000298
H	-3.103873	1.417415	-0.000768
C	-4.744739	-0.037996	-0.000260
H	-5.258317	0.401659	0.874155
H	-4.898801	-1.125748	-0.000153
H	-5.258454	0.401593	-0.874609

anethole

Geometry with 23 atoms:

Thermal correction to Gibbs Free Energy: 0.155642

Total energy: -463.329277376

H	-0.327962	-2.294881	0.000252
C	0.036128	-1.261477	0.000220
C	0.971736	1.342815	0.000155
C	-0.895071	-0.218253	0.000225
C	1.411609	-1.031176	0.000160
C	1.889051	0.281067	0.000121
C	-0.388046	1.095128	0.000210
H	2.095920	-1.882700	0.000164
H	-1.078653	1.944189	0.000258
H	1.367533	2.362194	0.000144
O	3.195635	0.622151	0.000068
C	4.154582	-0.393638	-0.000502
H	4.077911	-1.036390	0.896593
H	5.140647	0.089792	-0.000890
H	4.077071	-1.036156	-0.897690
H	-2.565302	-1.600858	0.000537
C	-2.325835	-0.526990	0.000224
C	-3.348437	0.339956	-0.000128
H	-3.134836	1.418157	-0.000415
C	-4.785213	-0.046067	-0.000355
H	-5.315260	0.357394	0.880276
H	-4.911143	-1.140275	0.001491
H	-5.314017	0.354149	-0.883242

[N(2,4,6-tribromophenyl)3]˙+

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.117401

Total energy: -23910.371532500

N	0.000070	0.000313	0.000628
C	-0.339684	1.362586	0.000597
C	-1.021171	4.094558	0.000179
C	0.294895	2.282132	-0.881721
C	-1.332035	1.876467	0.882510
C	-1.669747	3.219660	0.874567
C	-0.037765	3.626562	-0.874260
H	-2.421281	3.595749	1.572797
H	0.448914	4.311322	-1.572873
C	-1.009945	-0.975052	-0.000145
C	-3.037063	-2.930028	0.000345
C	-2.124753	-0.883957	-0.881068

C	-0.958765	-2.092755	0.880500
C	-1.954088	-3.055836	0.873237
C	-3.123350	-1.843707	-0.873330
H	-3.960261	-1.763430	-1.571161
C	1.349608	-0.386337	0.000749
C	4.057008	-1.161463	-0.000525
C	2.291200	0.216227	0.882349
C	1.828843	-1.395789	-0.881396
C	3.159679	-1.779374	-0.874466
C	3.623479	-0.162398	0.874071
H	3.509200	-2.543273	-1.573088
H	4.324869	0.300602	1.572337
Br	5.849946	-1.675232	-0.001652
Br	-1.471971	5.904507	0.000549
Br	0.356599	-2.290307	2.215852
Br	-2.271536	0.434470	-2.219736
Br	-2.154347	0.835671	2.221087
Br	1.509627	1.748907	-2.220312
Br	1.801794	1.447917	2.222263
Br	0.759975	-2.183129	-2.219034
H	-1.903536	-3.895561	1.570455
Br	-4.379416	-4.224992	0.000524

N(2,4,6-tribromophenyl)3

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.118178

Total energy: -23910.597624800

N	-0.002105	0.004064	-0.001024
C	-1.322519	0.518796	0.001310
C	-3.958244	1.542976	0.003480
C	-1.734006	1.521601	-0.903479
C	-2.301638	0.057017	0.907945
C	-3.606268	0.540026	0.897642
C	-3.022459	2.046273	-0.891356
H	-4.334094	0.151319	1.613471
H	-3.297739	2.824743	-1.606574
C	0.210739	-1.397656	0.001620
C	0.638005	-4.194535	0.004430
C	-0.465318	-2.257793	-0.891917
C	1.111280	-2.014861	0.897518
C	1.342641	-3.386796	0.887776
C	-0.275927	-3.636058	-0.879680
H	-0.822220	-4.264243	-1.586945
C	1.105329	0.889089	-0.005704
C	3.320738	2.648327	-0.007694
C	1.197290	1.975590	0.891978
C	2.182435	0.732618	-0.905607
C	3.285282	1.580751	-0.895335
C	2.273302	2.857428	0.880021
H	4.099183	1.420163	-1.605914
H	2.302354	3.686467	1.590766
Br	4.799332	3.819456	-0.007691
Br	-5.716871	2.224826	0.004066
Br	2.023263	-1.050767	2.245320
Br	-1.623083	-1.614603	-2.242217
Br	-1.908968	-1.192659	2.271632
Br	-0.600863	2.177835	-2.267484
Br	-0.083613	2.280206	2.249182
Br	2.190836	-0.590085	-2.257028
H	2.051751	-3.821805	1.595757
Br	0.923725	-6.058833	0.005618

[N(4-bromophenyl)3]·+

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.193925

Total energy: -8469.621496220

N	-0.002079	-0.000440	-0.001820
C	0.747833	-1.186413	-0.001632
C	2.235802	-3.538642	0.000888
C	0.325265	-2.289473	-0.767923
C	1.924794	-1.275958	0.765799
C	2.661891	-2.446443	0.768918
C	1.067135	-3.456974	-0.768319
H	3.564747	-2.528870	1.379174
H	0.755625	-4.308895	-1.377833
C	0.650689	1.241920	-0.002834
C	1.948372	3.704110	-0.001246
C	1.814696	1.426390	-0.773107
C	0.144101	2.305757	0.767672
C	0.791571	3.528094	0.770289
C	2.456949	2.651488	-0.774377
H	3.348790	2.806826	-1.386630
C	-1.403839	-0.055843	-0.000961
C	-4.184903	-0.165259	0.000173
C	-2.071222	-1.031162	0.764505
C	-2.146501	0.863980	-0.765919
C	-3.528413	0.806936	-0.767085
C	-3.453348	-1.082750	0.766750
H	-4.109417	1.504745	-1.375304
H	-3.977199	-1.824209	1.375182
H	0.415346	4.350871	1.383229
H	-1.495128	-1.725119	1.383270
H	-1.627156	1.601157	-1.384947
H	-0.741755	2.153035	1.390713
H	2.236391	-0.430152	1.385176
H	2.190839	0.609474	-1.395463
H	-0.571010	-2.209447	-1.389500
Br	2.820283	5.356257	0.001803

Br	-6.051215	-0.239131	0.000876
Br	3.234910	-5.116979	0.001210

N(4-bromophenyl)3

Geometry with 34 atoms:

Thermal correction to Gibbs Free Energy: 0.193465

Total energy: -8469.813644740

N	-0.000207	0.000892	0.003949
C	1.159659	0.805220	0.002823
C	3.456167	2.397271	-0.000122
C	2.256158	0.471681	-0.803088
C	1.233261	1.949984	0.807205
C	2.370771	2.748688	0.800563
C	3.403118	1.256656	-0.799330
H	2.422039	3.640245	1.431301
H	4.255009	0.991121	-1.431038
C	-1.276833	0.602827	0.002701
C	-3.805012	1.793283	0.000169
C	-1.537493	1.718495	-0.803644
C	-2.304369	0.093701	0.807729
C	-3.565318	0.678268	0.801295
C	-2.791418	2.318124	-0.799713
H	-2.988383	3.188045	-1.431965
C	0.116647	-1.405694	0.003036
C	0.348584	-4.190380	0.000171
C	1.070070	-2.041381	0.809107
C	-0.718737	-2.188776	-0.804329
C	-0.611661	-3.574508	-0.800642
C	1.193733	-3.425744	0.802518
H	-1.265975	-4.179647	-1.433848
H	1.939447	-3.915557	1.434408
H	-4.362468	0.276380	1.432411
H	1.721300	-1.438291	1.448923
H	-1.460641	-1.700507	-1.443346
H	-2.107846	-0.772443	1.446754
H	0.385148	2.213863	1.446137
H	-0.743790	2.118173	-1.441954
H	2.204702	-0.415856	-1.440879
Br	-5.516068	2.598906	-0.001839
Br	0.505958	-6.075015	-0.002021
Br	5.010652	3.474450	-0.001946

[NEt3]·+

Geometry with 22 atoms:

Thermal correction to Gibbs Free Energy: 0.168117

Total energy: -292.114113088

N	0.150483	0.017366	0.112630
C	-0.495705	-1.019505	-0.657058
H	-1.113360	-0.550328	-1.438964
H	0.293355	-1.611147	-1.148841
C	-1.351376	-1.907912	0.247886
H	-2.157268	-1.336942	0.732806
H	-0.741672	-2.392363	1.025262
H	-1.811085	-2.694913	-0.366345
C	-0.528022	1.231069	0.508871
H	0.243137	2.024871	0.538724
H	-0.804011	1.083527	1.578834
C	-1.723607	1.630344	-0.316592
H	-1.455343	1.797122	-1.371156
H	-2.118836	2.578436	0.073487
H	-2.541159	0.896046	-0.266220
C	1.498292	-0.203663	0.592136
H	1.610606	-1.281589	0.800521
H	1.620861	0.349211	1.538030
C	2.523410	0.255270	-0.442302
H	3.531519	0.070467	-0.045443
H	2.429718	1.331811	-0.649685
H	2.422212	-0.299386	-1.387066

NEt3

Geometry with 22 atoms:

Thermal correction to Gibbs Free Energy: 0.169802

Total energy: -292.298458075

N	0.000119	-0.306548	-0.004702
C	-1.209861	-1.079659	0.184214
H	-1.061969	-2.058030	-0.307393
H	-1.387816	-1.310558	1.264724
C	-2.438429	-0.418292	-0.403114
H	-2.289125	-0.212586	-1.475663
H	-2.672491	0.538845	0.091845
H	-3.323588	-1.063949	-0.292417
C	-0.000136	0.971489	0.698102
H	0.875239	1.026061	1.376306
H	-0.875267	1.025535	1.376681
C	-0.000652	2.168566	-0.232557
H	0.885151	2.156814	-0.887812
H	-0.000764	3.118787	0.326425
H	-0.886733	2.156393	-0.887424
C	1.210344	-1.079261	0.184300
H	1.062738	-2.057744	-0.307168
H	1.388402	-1.309963	1.264833
C	2.438675	-0.417587	-0.403184
H	3.324042	-1.062965	-0.292514
H	2.672494	0.539670	0.091659
H	2.289197	-0.212014	-1.475733

thianthrene

Geometry with 22 atoms:

Thermal correction to Gibbs Free Energy: 0.124914

Total energy: -1258.288342080

H	2.467451	2.486963	-0.318274
C	2.487669	1.392804	-0.300866
C	2.487666	-1.392805	-0.300872
C	1.369458	0.700739	0.171355
C	3.612729	0.696890	-0.733574
C	3.612728	-0.696892	-0.733578
C	1.369457	-0.700740	0.171353
H	4.489071	1.248263	-1.085283
H	4.489068	-1.248265	-1.085291
H	2.467446	-2.486964	-0.318285
S	0.000000	1.626870	0.822763
S	-0.000000	-1.626870	0.822764
C	-1.369457	0.700740	0.171353
C	-1.369458	-0.700740	0.171355
C	-2.487666	1.392805	-0.300871
H	-2.467445	2.486964	-0.318284
C	-2.487669	-1.392804	-0.300866
H	-2.467451	-2.486963	-0.318275
C	-3.612729	-0.696890	-0.733575
H	-4.489071	-1.248262	-1.085284
C	-3.612728	0.696892	-0.733577
H	-4.489068	1.248265	-1.085290

[thianthrenium]˙+

Geometry with 22 atoms:

Thermal correction to Gibbs Free Energy: 0.123799

Total energy: -1258.090914250

H	2.623911	-2.492605	-0.000008
C	2.627385	-1.397930	-0.000005
C	2.627382	1.397930	0.000037
C	1.400666	-0.707535	0.000073
C	3.820190	-0.702769	-0.000046
C	3.820189	0.702774	-0.000021
C	1.400664	0.707531	0.000089
H	4.765368	-1.250623	-0.000126
H	4.765367	1.250627	-0.000078
H	2.623900	2.492605	0.000065
S	-0.000001	-1.734698	-0.000036
S	0.000001	1.734696	-0.000038
C	-1.400664	-0.707532	0.000082
C	-1.400666	0.707535	0.000067
C	-2.627382	-1.397930	0.000034
H	-2.623904	-2.492605	0.000063
C	-2.627384	1.397931	-0.000004
H	-2.623907	2.492606	-0.000004
C	-3.820190	0.702771	-0.000043
H	-4.765368	1.250625	-0.000117
C	-3.820189	-0.702772	-0.000021
H	-4.765367	-1.250626	-0.000076

III-f-s

Geometry with 49 atoms:

Thermal correction to Gibbs Free Energy: 0.34196

Total energy: -2486.877238060

Ni	0.047998	-1.846776	-0.605517
C	2.127976	0.040981	-0.328454
C	3.342364	0.605930	0.056616
C	4.357256	-0.196256	0.581456
C	4.087684	-1.565569	0.703089
C	2.853590	-2.058164	0.309500
C	1.009162	0.812360	-0.905112
C	0.993008	2.202232	-1.017244
C	-0.119903	2.842491	-1.567582
C	-1.175364	2.033263	-2.005918
C	-1.089299	0.657064	-1.850581
H	3.508534	1.680864	-0.056162
H	4.839615	-2.246395	1.111752
H	2.615752	-3.122906	0.407209
H	1.839878	2.798461	-0.665832
H	-2.068884	2.478466	-2.452906
H	-1.910790	-0.000189	-2.161340
N	1.887266	-1.282522	-0.197767
N	-0.028486	0.057945	-1.309795
C	5.679804	0.371876	0.975351
H	6.432097	0.177208	0.192265
H	5.628982	1.460260	1.121722
H	6.055648	-0.092822	1.899490
C	-0.200134	4.330108	-1.658671
H	-0.863344	4.725816	-0.870597
H	0.784597	4.802329	-1.533103
H	-0.626595	4.650059	-2.621633
C	-1.698124	-2.766024	-0.635496
N	-2.774055	-2.052732	0.079235
H	-2.023158	-2.838751	-1.699665
H	-1.679078	-3.824273	-0.289277
C	-2.514088	-0.878752	0.763562
C	-4.098654	-2.259731	-0.435663
C	-3.393143	0.221314	0.762780
C	-1.323690	-0.733920	1.516816
H	-4.236710	-3.329690	-0.660954
H	-4.876247	-1.970516	0.292184
H	-4.299458	-1.700220	-1.378742
C	-3.057764	1.416452	1.404815
H	-4.336145	0.171062	0.211312
C	-1.003535	0.460078	2.142478
H	-0.651496	-1.593709	1.604103

C	-1.852348	1.578479	2.088330
H	-3.757790	2.259384	1.349393
H	-0.060844	0.531340	2.701419
C	-1.459958	2.876654	2.726101
H	-0.583477	3.327637	2.226269
H	-2.276948	3.613653	2.682861
H	-1.180190	2.748642	3.785956

III'-f-s

Geometry with 50 atoms:

Thermal correction to Gibbs Free Energy: 0.345767

Total energy: -5061.019636710

Ni	1.444367	-0.703806	0.401225
Br	3.716186	-0.177573	0.602288
C	-1.205172	-0.447936	1.221705
C	-2.510652	-0.780288	1.562112
C	-2.915548	-2.117735	1.570601
C	-1.945952	-3.076240	1.261420
C	-0.663551	-2.671509	0.919046
C	-0.688576	0.929968	1.199636
C	-1.497386	2.059461	1.203319
C	-0.919102	3.329224	1.108012
C	0.475571	3.392288	1.045667
C	1.219575	2.217767	1.058188
H	-3.222766	0.005107	1.831120
H	-2.190538	-4.141555	1.274926
H	0.099031	-3.407677	0.646702
H	-2.586816	1.960608	1.236193
H	0.985139	4.357360	0.977239
H	2.314765	2.229026	0.999334
N	-0.297588	-1.387568	0.876371
N	0.656564	1.010780	1.128177
C	-4.327976	-2.490811	1.868559
H	-4.757878	-1.849880	2.652598
H	-4.950195	-2.355020	0.966847
H	-4.417389	-3.542185	2.176149
C	-1.775426	4.548183	1.032958
H	-2.317563	4.571052	0.072027
H	-2.538945	4.548360	1.826287
H	-1.184436	5.471234	1.110740
C	1.664120	-1.831933	-1.124644
N	1.300094	-0.878438	-2.153926
H	2.687479	-2.190301	-1.316985
H	0.982768	-2.700565	-1.129354
C	-0.014863	-0.400541	-2.198972
C	2.343422	-0.019866	-2.658903
C	-0.307826	0.966905	-2.338855
C	-1.103172	-1.285111	-2.073193
H	3.267366	-0.604621	-2.780694
H	2.059493	0.383417	-3.644431
H	2.588288	0.830401	-1.989095
C	-1.622816	1.425295	-2.271140
H	0.500391	1.695782	-2.443683
C	-2.405874	-0.813317	-2.007380
H	-0.916088	-2.360710	-2.005669
C	-2.698908	0.556403	-2.078905
H	-1.810430	2.504466	-2.335112
H	-3.226655	-1.530349	-1.879289
C	-4.104357	1.055262	-1.936783
H	-4.629174	0.539807	-1.114028
H	-4.127983	2.136427	-1.726574
H	-4.703330	0.885227	-2.848643

III-f-TS

Geometry with 64 atoms:

Thermal correction to Gibbs Free Energy: 0.447315

Total energy: -5331.796353960

Ni	-0.750465	-0.560632	-0.110381
C	-2.431531	-1.540971	-0.123475
C	-4.947208	-0.251661	-0.190472
C	-3.320407	-1.660578	0.972548
C	-2.883838	-0.915690	-1.309808
C	-4.108836	-0.237894	-1.303561
C	-4.529349	-0.995166	0.939367
H	-3.012504	-2.218567	1.863748
H	-2.279676	-0.959363	-2.222708
H	-4.428798	0.290240	-2.209725
H	-5.186408	-1.039145	1.816651
N	-1.052179	1.473228	-0.100261
C	-1.031307	4.258550	0.124095
C	-2.076248	2.116584	0.465997
C	-0.006537	2.179127	-0.566369
C	0.030015	3.572872	-0.464726
C	-2.110473	3.495268	0.595602
N	0.811478	0.055536	-1.282119
C	3.302999	1.073321	-2.058309
C	1.744171	-0.741643	-1.811152
C	1.078754	1.372278	-1.155218
C	2.315148	1.902885	-1.526879
C	2.983604	-0.280723	-2.224316
H	-2.900685	1.490045	0.829697
H	0.884733	4.134134	-0.851558
H	-2.971066	3.979923	1.065208
H	1.482576	-1.803655	-1.893036
H	2.525518	2.966416	-1.384702
H	3.711324	-0.977438	-2.650502
Br	-1.200406	-3.224314	-0.540261
C	4.661529	1.592218	-2.390332

H	4.653372	2.675638	-2.578022
H	5.348748	1.408857	-1.545503
H	5.087125	1.080365	-3.266448
C	-1.034151	5.745757	0.248837
H	-1.143200	6.049998	1.302234
H	-0.111363	6.192768	-0.146546
H	-1.888720	6.181582	-0.293788
C	-0.379547	-0.724186	1.843015
N	0.799181	0.029787	2.221846
H	-1.239384	-0.313063	2.401394
H	-0.275014	-1.787958	2.138178
C	2.052905	-0.377930	1.832189
C	0.635130	1.352652	2.765142
C	3.189036	0.452070	1.972276
C	2.263876	-1.656170	1.257511
H	-0.410475	1.494619	3.070416
H	1.266887	1.510607	3.658343
H	0.887045	2.157228	2.042615
C	4.443907	0.031208	1.540584
H	3.093987	1.450153	2.406352
C	3.527508	-2.053374	0.843142
H	1.418372	-2.331563	1.108449
C	4.650074	-1.223144	0.958083
H	5.295715	0.713013	1.655865
H	3.644349	-3.046912	0.391436
C	5.992842	-1.654820	0.450287
H	6.015408	-1.715446	-0.653106
H	6.784908	-0.951865	0.752567
H	6.272970	-2.655129	0.821798
C	-6.266909	0.455864	-0.181787
H	-7.106356	-0.241215	-0.014678
H	-6.320352	1.205152	0.627320
H	-6.452089	0.979187	-1.132048

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